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Host Materials for Transition-Metal Ions

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Data are given on host materials for lasers that use the transition-metal ions. Included in each section are the crystallographic data, x-ray data, crystal-field components A_{nm}, crystal field parameters B_{nm} (Dq), and spin-orbit constants (ζ). One section contains the phenomenological free-ion parameters $F^{(k)}$, ζ, and α, which have been obtained by fitting the reported free-ion data. There is a bibliography for each host which, depending on the host, is more or less complete. The data contained on each host material will be updated periodically, and data on new host materials will be added.

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TABLES

1. Introduction

This report contains information on various potential laser host materials for transition-metal ions of the nd^N electronic configuration. The list is an update of a previous report [1] with a number of new materials added. Many of the new host materials have been reported as practical laser systems, employing transition-metal ions as well as rare-earth ions. Frequently the decision for the inclusion of a particular host material was made on the grounds that the material had some particular interesting feature in addition to being a potential laser host.

Extensive data on the free-ion parameters for the $3d^N$ electronic configuration have been reported, and these are given in table 1 for the doubly, triply, and quadruply ionized states. Also included in table 1 are the parameters of the $4d^N$ and $5d^N$ electronic configurations; a considerable number of these latter configurations have not been investigated. Nonrelativistic Hartree-Fock values for $F^{(k)}$, ζ, and $\langle r^k \rangle$ for the doubly, triply, and quadruply ionized states of the $3d^N$, $4d^N$, and $5d^N$ electronic configurations are given in table 2.

A number of host materials were selected because lasers had been reported employing $3d^N$ ions as impurities. These host materials with limited amounts of experimental energy levels were reported during the early 1960's, and some later work has been done in some of these hosts. Unfortunately, much of the reported absorption data have been taken at room temperature (~300 K) and are quite unreliable because of the presence of vibronics and absorption from excited levels. Further complications arise when the data are extracted from the excitation spectra. There is a real need for low-temperature absorption spectra of many of these ions.

TABLE 1. FREE-ION DATA: $F^{(2)}$, $F^{(4)}$, ζ, and α for nd^N ions (cm^{-1})
(A) $3d^N$

nd^N	Ion	$F^{(2)}$	$F^{(4)}$	ζ	α	Reference
$3d^1$	Sc^{2+}	--	--	79.06	--	--
$3d^1$	Ti^{3+}	--	--	152.84	--	--
$3d^1$	V^{4+}	--	--	249.95	--	--
$3d^2$	Sc^{1+}	35,469	19,832	63.18	27	4
$3d^2$	Ti^{2+}	53,061	30,920	126.4	56.4	4
$3d^2$	Ti^{2+}	54,870	32,034	129.4	20.80	5
$3d^2$	Ti^{2+}	53,322[a]	29,000[a]	120.4[b]	--	1
$3d^2$	Ti^{2+}	54,927	32,206	118.0	20.52	9
$3d^2$	V^{3+}	67,200	40,522	219.6	75	4
$3d^2$	V^{3+}	69,547	42,234	206.0	27.54	9
$3d^2$	Cr^{4+}	75,831	47,061	337.9	--	4
$3d^2$	Cr^{4+}	82,406	50,755	319.0	37.64	9
$3d^3$	V^{2+}	55,153	20,954	186.3	199	4
$3d^3$	V^{2+}	59,669	35,882	176.7	24.58	5
$3d^3$	V^{2+}	57,437[a]	36,363[a]	167.8[b]	--	7
$3d^3$	V^{2+}	59,924	36,268	170.0	22.90	9
$3d^3$	Cr^{3+}	75,950	30,076	295.6	437	4
$3d^3$	Cr^{3+}	70,905[a]	45,986[a]	296.4[b]	--	8
$3d^3$	Cr^{3+}	74,201	45,822	275.0	29.87	9
$3d^3$	Mn^{4+}	80,332	47,754	437.0	91	4
$3d^3$	Mn^{4+}	86,939	54,219	405.0	39.01	9
$3d^4$	Cr^{2+}	59,121[a]	46,179[a]	234.3[b]	--	8
$3d^4$	Cr^{2+}	62,300	38,934	263.2	61.0	4
$3d^4$	Cr^{2+}	64,467	39,730	239.4	28.36	5
$3d^4$	Cr^{2+}	64,798	40,288	231.0	25.83	9
$3d^4$	Mn^{3+}	81,970	46,998	387.7	12	4
$3d^4$	Mn^{3+}	71,593[a]	55,647[a]	361.8[b]	--	2
$3d^4$	Mn^{3+}	78,756	49,404	--	32.60	9
$3d^4$	Fe^{4+}	87,269	56,183	564.6	85	4
$3d^4$	Fe^{4+}	91,372	57,696	513.0	40.66	9

TABLE 1 (cont'd). FREE-ION DATA: $F^{(2)}$, $F^{(4)}$, ζ, and α for nd^N ions (cm^{-1})
(A) $3d^N$ (cont'd)

nd^N	Ion	$F^{(2)}$	$F^{(4)}$	ζ	α	Reference
$3d^5$	Mn^{2+}	67,685	40,698	351.4	74.8	3
$3d^5$	Mn^{2+}	69,266	43,578	317.5	32.14	5
$3d^5$	Mn^{2+}	69,485	44,305	316.0	29.20	9
$3d^5$	Fe^{3+}	83,302	53,070	463.0	35.40	9
$3d^5$	Co^{4+}	95,819	61,152	654.0	42.68	9
$3d^6$	Fe^{2+}	79,149	49,153	440.5	81	4
$3d^6$	Fe^{2+}	74,064	47,426	411.0	35.92	5
$3d^6$	Fe^{2+}	74,282	48,241	422.0	33.21	9
$3d^6$	Co^{3+}	84,377[a]	60,291[a]	584.6[b]	--	6
$3d^6$	Co^{3+}	87,762	56,823	606.0	37.93	9
$3d^6$	Ni^{4+}	100,186	64,788	830.0	44.17	9
$3d^7$	Co^{2+}	77,532	50,123	560.3	65	4
$3d^7$	Co^{2+}	78,906	52,277	536.0	37.48	9
$3d^7$	Co^{2+}	78,863	51,274	519.9	39.70	5
$3d^7$	Ni^{3+}	92,204	60,579	749.0	41.01	9
$3d^7$	Cu^{4+}	104,534	68,395	1008	46.40	9
$3d^8$	Ni^{2+}	86,933	60,871	701.7	42	4
$3d^8$	Ni^{2+}	83,661	55,122	644.2	43.48	5
$3d^8$	Ni^{2+}	83,514	56,164	668.0	42.49	9
$3d^8$	Cu^{3+}	96,631	64,302	911.0	44.79	9
$3d^8$	Zn^{4+}	108,877	71,954	1203.0	49.84	9
$3d^9$	Cu^{2+}	--	--	828.68	--	--
$3d^9$	Zn^{3+}	--	--	--	--	--
$3d^9$	Ga^{4+}	--	--	--	--	--

[a]The Slater parameters are obtained by fitting the centroids of the reported experimental data for a given nd^N configuration.
[b]The ζ values are obtained by fitting the lowest J multiple of the Hund ground state of the nd^N configuration.

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The parameters are given in the form

$$F^{(2)} = 69{,}266 + 4798.5(N - 5)$$

$$F^{(4)} = 43{,}578 + 3848(N - 5)$$

$$\alpha = 32.14 + 3.78(N - 5)$$

$$\zeta = 348.3 + 85.8(N - 5) + 7.7[(N - 5)^2 - 4]$$

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TABLE 1 (cont'd). FREE-ION DATA: $F^{(2)}$, $F^{(4)}$, ζ, and α nd^N ions (cm^{-1})
(B) $4d^N$

$4d^N$	Ion	$F^{(2)}$	$F^{(4)}$	ζ	α	Reference
$4d^1$	Y^{2+}	--	--	289.92	--	1
$4d^1$	Zr^{3+}	--	--	500.24	--	2
$4d^1$	Nb^{4+}	--	--	742.16	--	3
$4d^2$	Zr^{2+}	34,790	23,373	--	--	4
$4d^2$	Zr^{2+}	38,721	19,498	408.47	89.94	5
$4d^2$	Zr^{2+}	37,170	20,160	450	25	6
$4d^2$	Nb^{3+}	47,297	31,781	646.64	--	7
$4d^2$	Mo^{4+}	54,755	35,818	920.64	44.48	8
$4d^3$	Nb^{2+}	39,950	26,901	--	--	4
$4d^3$	Nb^{2+}	41,517	25,427	535	33	6
$4d^3$	Mo^{3+}	50,411	32,830	810	38	9
$4d^3$	Tc^{4+}	--	--	--	--	--
$4d^4$	Mo^{2+}	45,080	30,429	--	--	4
$4d^4$	Tc^{3+}	--	--	--	--	--
$4d^4$	Ru^{4+}	--	--	--	--	--
$4d^5$	Tc^{2+}	50,225	33,957	--	--	4
$4d^5$	Ru^{3+}	--	--	--	--	--
$4d^5$	Rh^{4+}	--	--	--	--	--
$4d^6$	Ru^{2+}	55,370	37,485	--	--	4
$4d^6$	Rh^{3+}	--	--	--	--	--
$4d^6$	Pd^{4+}	--	--	--	--	--
$4d^7$	Rh^{2+}	60,515	41,013	--	--	4
$4d^7$	Rh^{2+}	54,117	38,582	1291	29	6
$4d^7$	Pd^{3+}	61,943	43,516	1699.1	31.6	10
$4d^7$	Ag^{4+}	71,497	51,108	2289	32.2	11
$4d^8$	Pd^{2+}	65,660	44,541	--	--	4
$4d^8$	Pd^{2+}	57,302	41,933	1545	28	6
$4d^8$	Pd^{2+}	57,766	42,591	1551	21.9	12
$4d^8$	Ag^{3+}	65,305	46,002	1996.04	45.98	13
$4d^8$	Cd^{4+}	72,155	50,707	2494.91	47.78	14
$4d^9$	Ag^{2+}	--	--	1843.68	--	15
$4d^9$	Ag^{2+}	--	--	1825	--	6
$4d^9$	Cd^{3+}	--	--	2325	--	16
$4d^9$	La^{4+}	--	--	--	--	--

References for part B, $4d^N$ ions

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TABLE 1 (cont'd). FREE-ION DATA: $F^{(2)}$, $F^{(4)}$, ζ, and α for nd^N ions (cm^{-1})
(C) $5d^N$

$5d^N$	Ion	F^2	F^4	ζ	α	Reference
$5d^1$	Lu^{2+}	-- --	1,176.08	--	1	--
$5d^1$	Hf^{3+}	-- --	1,876.8	--	2	--
$5d^1$	Ta^{4+}	-- --	2,643.32	--	3	--
$5d^2$	Hf^{2+}	-- --	--	--	--	--
$5d^2$	Ta^{3+}	45,551	28,658	22,813	66.22	4
$5d^2$	W^{4+}	52,112	34,335	3,102	--	9
$5d^3$	Ta^{2+}	-- --	--	--	--	--
$5d^3$	W^{3+}	47,530	29,988	2,720	25	10
$5d^3$	Re^{4+}	-- --	--	--	--	--
$5d^4$	W^{2+}	-- --	--	--	--	--
$5d^4$	Re^{3+}	-- --	--	--	--	--
$5d^4$	Os^{4+}	-- --	--	--	--	--
$5d^5$	Re^{2+}	30,870	22,050	--	--	--
$5d^5$	Os^{3+}	-- --	--	--	--	--
$5d^5$	Ir^{4+}	-- --	--	--	--	--
$5d^6$	Os^{2+}	30,135	18,963	1,900	3200	6
$5d^6$	Ir^{3+}	-- --	--	--	--	--
$5d^6$	Pt^{4+}	-- --	--	--	--	--
$5d^7$	Ir^{2+}	-- --	--	--	--	--
$5d^7$	Pt^{3+}	-- --	--	--	--	--
$5d^7$	Au^{4+}	-- --	--	--	--	--
$5d^8$	Pt^{2+}	-- --	--	--	--	--
$5d^8$	Au^{3+}	-- --	--	--	--	--
$5d^8$	Hg^{4+}	-- --	--	--	--	--
$5d^9$	Au^{2+}	-- --	5,078	--	11	--
$5d^9$	Hg^{3+}	-- --	6,274	--	11	--
$5d^9$	Tl^{4+}	-- --	--	--	--	--

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TABLE 2. HARTREE-FOCK VALUES FOR $F^{(k)}$, ζ, AND $\langle r^k \rangle$ FOR nd^N IONS

(A) $3d^N$

Z	X^{2+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ_d (cm^{-1})	$\langle r^2 \rangle$ (Å^2)	$\langle r^4 \rangle$ (Å^4)
21	Sc	$3d^1$	--	--	85.95	0.8346	1.4997
22	Ti	$3d^2$	67,932	42,357	131.15	0.6716	0.9808
23	V	$3d^3$	74,062	46,171	187.17	0.5677	0.7112
24	C	$3d^4$	79,790	49,726	256.60	0.4910	0.5401
25	Mn	$3d^5$	85,637	53,368	342.85	0.4277	0.4145
26	Fe	$3d^6$	89,877	55,927	441.38	0.3893	0.3527
27	Co	$3d^7$	94,600	58,817	561.21	0.3525	0.2949
28	Ni	$3d^8$	99,392	61,756	703.19	0.3203	0.2478
29	Cu	$3d^9$	--	--	869.65	0.2923	0.2097

Z	X^{3+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ_d (cm^{-1})	$\langle r^2 \rangle$ (Å^2)	$\langle r^4 \rangle$ (Å^4)
22	Ti	$3d^1$	--	--	157.75	0.5341	0.5769
23	V	$3d^2$	82,940	52,097	220.47	0.4571	0.4270
24	Cr	$3d^3$	88,514	55,558	296.26	0.4018	0.3344
25	Mn	$3d^4$	93,852	58,861	388.01	0.3578	0.2688
26	Fe	$3d^5$	99,367	62,291	499.53	0.3196	0.2168
27	Co	$3d^6$	103,474	64,758	625.26	0.2947	0.1884
28	Ni	$3d^7$	108,043	67,546	775.62	0.2705	0.1615
29	Cu	$3d^8$	112,696	70,392	951.32	0.2489	0.1389
30	Zn	$3d^9$	--	--	1154.85	0.2297	0.1200

Z	X^{4+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ_d (cm^{-1})	$\langle r^2 \rangle$ (Å^2)	$\langle r^4 \rangle$ (Å^4)
23	V	$3d^1$	--	--	253.27	0.4398	0.6494
24	Cr	$3d^2$	96,286	60,775	337.03	0.3708	0.4203
25	Mn	$3d^3$	101,615	64,078	436.20	0.3568	0.4097
26	Fe	$3d^4$	106,766	67,260	554.03	0.2914	0.2686
27	Co	$3d^5$	112,112	70,581	694.80	0.2721	0.2271
28	Ni	$3d^6$	116,164	73,011	851.77	0.2497	0.1875
29	Cu	$3d^7$	120,659	75,748	1036.93	0.2283	0.1524
30	Zn	$3d^8$	125,241	78,548	1250.84	0.2100	0.1200
31	Ca	$3d^9$	--	--	1496.12	0.1800	0.0800

TABLE 2 (cont'd). HARTREE-FOCK VALUES FOR $F^{(k)}$, ζ, AND $\langle r^k \rangle$ FOR nd^N IONS

(B) $4d^N$

Z	X^{2+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ (cm^{-1})	$\langle r^2 \rangle$ ($Å^2$)	$\langle r^4 \rangle$ ($Å^4$)
39	Y	$4d^1$	--	--	312	1.5737	4.4402
40	Zr	$4d^2$	51,177	33,321	432	1.2734	2.8974
41	Nb	$4d^3$	55,683	36,328	566	1.0769	2.0761
42	Mo	$4d^4$	59,873	39,117	718	0.9316	1.5580
43	Tc	$4d^5$	64,052	41,911	891	0.8145	1.1907
44	Ru	$4d^6$	67,247	43,978	1082	0.7365	0.9869
45	Rh	$4d^7$	70,673	46,224	1299	0.6656	0.8126
46	Pd	$4d^8$	74,108	48,480	1544	0.6045	0.6744
47	Ag	$4d^9$	--	--	1820	0.5516	0.5644

Z	X^{3+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ (cm^{-1})	$\langle r^2 \rangle$ ($Å^2$)	$\langle r^4 \rangle$ ($Å^4$)
40	Zr	$4d^1$	--	--	510	1.0840	1.989
41	Nb	$4d^2$	60,253	36,327	655	0.9288	1.461
42	Mo	$4d^3$	64,276	42,326	815	0.8149	1.128
43	Tc	$4d^4$	68,116	44,878	997	0.7244	0.8953
44	Ru	$4d^5$	72,001	47,470	1201	0.6479	0.7175
45	Rh	$4d^6$	75,061	49,443	1426	0.5936	0.6094
46	Pd	$4d^7$	78,342	51,586	1680	0.5435	0.5147
47	Ag	$4d^8$	81,645	53,754	1964	0.4993	0.4372
48	Cd	$4d^9$	--	--	2283	0.4603	0.3736

Z	X^{4+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ (cm^{-1})	$\langle r^2 \rangle$ ($Å^2$)	$\langle r^4 \rangle$ ($Å^4$)
41	Nb	$4d^1$	--	--	742	0.8715	1.559
42	Mo	$4d^2$	68,068	54,102	914	0.7520	1.085
43	Tc	$4d^3$	71,843	47,615	1105	0.7039	0.9993
44	Ru	$4d^4$	75,495	50,038	1319	0.5959	0.6777
45	Rh	$4d^5$	79,206	52,512	1557	0.5522	0.5776
46	Pd	$4d^6$	82,196	54,434	1820	0.5071	0.4823
47	Ag	$4d^7$	85,389	56,519	2114	0.4654	0.4005
48	Cd	$4d^8$	88,615	58,631	2441	0.4200	0.3200
49	In	$4d^9$	--	--	2806	0.3800	0.2400

TABLE 2 (cont'd). HARTREE-FOCK VALUES FOR $F^{(k)}$, ζ, AND $\langle r^k \rangle$ FOR nd^N IONS

(C) $5d^N$

Z	X^{2+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ (cm^{-1})	$\langle r^2 \rangle$ (Å^2)	$\langle r^4 \rangle$ (Å^2)
71	Lu	$5d^1$	-	-	1391	1.6197	4.6324
72	Hf	$5d^2$	50,350	33,000	1774	1.3646	3.2437
73	Ta	$5d^3$	54,008	35,526	2170	1.1926	2.4612
74	W	$5d^4$	57,369	37,840	2594	1.0610	1.9385
75	Re	$5d^5$	60,702	40,149	3053	0.9510	1.5467
76	Os	$5d^6$	63,123	41,766	3531	0.8779	1.3277
77	Ir	$5d^7$	65,755	43,550	4056	0.8087	1.1289
78	Pt	$5d^8$	68,388	45,344	4626	0.7474	0.9649
79	Au	$5d^9$	-	-	5248	0.6930	0.6646

Z	X^{3+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ (cm^{-1})	$\langle r^2 \rangle$ (Å^2)	$\langle r^4 \rangle$ (Å^2)
72	Hf	$5d^1$	-	-	2072	1.1760	2.2810
73	Ta	$5d^2$	58,176	38,604	2489	1.0420	1.7780
74	W	$5d^3$	61,293	40,754	2926	0.9399	1.4440
75	Re	$5d^4$	64,247	42,789	3394	0.8563	1.1960
76	Os	$5d^5$	67,234	44,856	3898	0.7829	0.9968
77	Ir	$5d^6$	69,479	46,349	4430	0.7309	0.8745
78	Pt	$5d^7$	71,922	48,001	5011	0.6809	0.7612
79	Au	$5d^8$	74,389	49,674	5640	0.6356	0.6646
80	Hg	$5d^9$	-	-	6323	0.5948	0.5826

Z	X^{4+}	nd^N	$F^{(2)}$ (cm^{-1})	$F^{(4)}$ (cm^{-1})	ζ (cm^{-1})	$\langle r^2 \rangle$ (Å^2)	$\langle r^4 \rangle$ (Å^2)
73	Ta	$5d^1$	-	-	2797	0.9823	1.8522
74	W	$5d^2$	64,633	43,252	3257	0.8727	1.3654
75	Re	$5d^3$	67,469	45,208	3741	0.8339	1.2966
76	Os	$5d^4$	70,197	47,082	4259	0.7247	0.9217
77	Ir	$5d^5$	72,980	49,004	4814	0.6841	0.8141
78	Pt	$5d^6$	75,122	50,424	5404	0.6393	0.7024
79	Au	$5d^7$	77,448	51,994	6045	0.5969	0.6030
80	Hg	$5d^8$	79,808	53,587	6736	0.5500	0.5000
81	Tl	$5d^9$	-	-	7486	0.5100	0.4000

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2. Presentation of Data

Each host is described in a series of tables organized as follows.

2.1 Crystallographic Data

The crystallographic data on each host are given in the notation of the International Tables [2]. The crystallographic data are presented in a short table for each host that lists the following information:

(a) The crystal class: triclinic, orthorhombic, etc.

(b) The space group symbol and number from the International Tables.

(c) The number of chemical formula units, Z, per unit cell.

(d) The setting, if there is more than one for that space group in the International Tables.

(e) The position (site type in the International Tables), site symmetry (in the Schoenflies notation), and general x, y, and z coordinates (expressed as fractions of the lattice constants) for that site type, for each constituent of the host crystal.

(f) The lattice constants a, b, and c (in angstroms) and angles α, β, and γ (in degrees and decimal parts).

(g) The effective charges (usually the valence charge) in units of the electronic charge.

(h) The electric-dipole polarizabilities, α (in $Å^3$), for each of the constituent ions.

2.2 Crystal-Field Components, A_{nm}, and Parameters, B_{nm}

For each host, the data described in section 2.1 were used to obtain the point-charge [3,4], point-dipole [5], and self-induced [6] contributions to the crystal-field components, A_{nm}. All the A_{nm} for $1 \le n \le 5$ are given and are sufficient for the analysis of the nd^N configuration. The units of A_{nm} are $cm^{-1}/Å^n$. The crystal-field parameters for a particular ion are given by $B_{nm} = \langle r^n \rangle A_{nm}$, where $\langle r^n \rangle$ is the radial expectation value [7] of r^n for the ion under consideration. At the bottom of a number of the tables of A_{nm}, the sums $S^{(0)}$, $S^{(2)}$, and $S^{(4)}$ are given.

The $S^{(0)}$ sum yields the interconfiguration shift [8]

$$\Delta E = \Delta E_0 - [\langle r^2\rangle_{n'\ell'} - \langle r^2\rangle_{n\ell}]S^{(0)},$$

and the $S^{(k)}$ sums yield the Slater integral shifts as $\Delta F^{(2)} = -\langle r^2\rangle^2 S^{(2)}$ and $\Delta F^{(4)} = -\langle r^4\rangle^2 S^{(4)}$; the units are such that if $\langle r^k\rangle$ is in angstrom units, then each shift is in units of cm^{-1}.

2.3 Experimental Results

For each host we include tables reporting all the experimental data in terms of the Slater integrals, $F^{(k)}$, and the crystal-field parameters, B_{nm}. Since there are a number of different notations we here describe in some detail our conversion from each set of constants to B_{nm} or $F^{(k)}$.

2.3.1 Relation of Dq with B_{40}

McClure [9] in his article gives the electric potential for a sixfold cubic array of charges at a distance R as

$$V = D[x^4 + y^4 + z^4 - \frac{3}{5} r^4] \quad , \tag{1}$$

where $D = 35e/4R^5$. The potential energy (in electron-volts) can be written as

$$U = eDr^4(X^4 + Y^4 + Z^4 - \frac{3}{5}) \quad , \tag{2}$$

where $X = x/r$, $Y = y/r$, and $Z = z/r$. For equivalent electrons McClure [9] defines q by $q = 2\langle r^4\rangle e/105$, so that

$$U = \frac{105}{2} Dq(X^4 + Y^4 + Z^4 - \frac{3}{5}) \quad . \tag{3}$$

In our notation we write the same potential as

$$U = B_{40}[C_{40} + \frac{5}{\sqrt{70}} (C_{44} + C_{4-4})] \quad , \tag{4}$$

for sixfold cubic coordination with charges at $(\pm R,0,0)$, $(0,\pm R,0)$, and $(0,0,\pm R)$. The C_{nm} are given by [8]

$$C_{40} = (35Z^4 - 30Z^2 + 3)/8 \quad , \tag{5}$$

$$C_{4\pm4} = (X \pm iY)^4(35/128)^{1/2} \quad . \tag{6}$$

Substituting (5) and (6) into (4) gives

$$C_{40} + \frac{5}{\sqrt{70}} (C_{44} + C_{4-4}) = \frac{5}{2} (X^4 + Y^4 + Z^4 - \frac{3}{5}) \quad . \tag{7}$$

Thus, we obtain

$$\frac{5}{2} B_{40} = \frac{105}{2} Dq \quad ,$$

or

$$B_{40} = 21 Dq \quad , \tag{8}$$

$$B_{44} = \sqrt{5/14}\ |B_{40}| \quad .$$

This relation (8) has been used to convert the Dq reported in the literature to B_{40}.

If, in the cubic group, the principal axis of rotation is the cube diagonal, then the crystal-field interaction is

$$H_{CEF} = B_{40} \sum_{i=1}^{N} C_{40}(i) + B_{43} \sum_{i=1}^{N} [C_{43}(i) - C_{4-3}(i)]$$

with $B_{40} = 14$ Dq,

$$B_{43} = \sqrt{10/7}\ |B_{40}| \quad . \tag{9}$$

If we write the cubic field parameter in equation (9) as $B_{40}^{(3)}$ and the cubic field parameter in equation (8) as $B_{40}^{(4)}$, then for the same crystal field in the two descriptions we have

$$B_{40}^{(3)} = -\frac{2}{3} B_{40}^{(4)} \quad . \tag{10}$$

For a crystal field of low symmetry, the correlation of the various notations used in the analysis of the crystal-field interaction is extremely difficult, and we shall not attempt to be complete here. Instead we shall relate what appears to be the most prevalent. For a crystal field of C_4 and higher symmetry, we write the crystal-field interaction as

$$H_{CEF} = B_{20} \sum_{i=1}^{N} C_{20}(i) + B_{40} \sum_{i=1}^{N} C_{40}(i) + B_{44} \sum_{i=1}^{N} [C_{44}(i) + C_{4-4}(i)] \quad , \tag{11}$$

where

$$C_{kq}(i) = \sqrt{4\pi/(2k+1)}\ Y_{kq}(\theta_i,\phi_i)$$

and all B_{kq} can be taken real.

The matrix elements of equation (11) for a single electron are given by [11]

$$\langle 20|H_{CEF}|20\rangle = \frac{2}{7} B_{20} + \frac{2}{7} B_{40} ,$$

$$\langle 2\pm1|H_{CEF}|2\pm1\rangle = \frac{1}{7} B_{20} - \frac{4}{21} B_{40} , \qquad (12)$$

$$\langle 2\pm2|H_{CEF}|2\pm2\rangle = \frac{-2}{7} B_{20} + \frac{1}{21} B_{40} ,$$

$$\langle 2\pm2|H_{CEF}|2\mp2\rangle = \frac{\sqrt{70}}{21} B_{44} ,$$

where $|2m\rangle = Y_{2m}$, $\langle 2m'|C_{kq}|2m\rangle = \int Y^*_{2m'} C_{kq} Y_{2m}\, d\Omega$, $d\Omega = \sin\theta\, d\theta\, d\phi$, and all the arguments of Y_{2m} and C_{kq} are θ and ϕ.

Ballhausen [10] (p 101) gives the corresponding matrix element for tetragonal fields in terms of Dq, Ds, and Dt. Thus, the following relations exist:

$$B_{20} = -7Ds ,$$

$$B_{40} = -14Ds - 21Dt , \qquad (13)$$

$$B_{44} = \frac{3}{2}\sqrt{70}\, Dq .$$

By comparing the matrix elements of Griffith [12] for tetragonal symmetry we obtain

$$B_{20} = \delta - \mu ,$$

$$B_{40} = 21Dq - \left(\delta + \frac{3\mu}{4}\right) , \qquad (14)$$

$$B_{44} = \left(\frac{3\sqrt{70}}{10}\right)Dq + \left(\delta + \frac{3\mu}{4}\right)\frac{\sqrt{70}}{10} .$$

For C_3 and higher symmetry we write the crystal field for the electronic configuration d^N as

$$H_{CEF} = B_{20} \sum_{i=1}^{N} C_{20}(i) + B_{40} \sum_{i=1}^{N} C_{40}(i) + B_{43} \sum_{i=1}^{N} \left[C_{43}(i) - C_{4-3}(i)\right] . \qquad (15)$$

The matrix elements of the first two terms of (15) are the same as in (12) above and

$$\langle 2-2|H_{CEF}|21\rangle = \frac{\sqrt{35}}{21} B_{43} . \qquad (16)$$

By comparing the matrix elements for trigonal symmetry of Ballhausen [10] (p 104) we obtain

$$
\begin{aligned}
B_{20} &= -7D\sigma \quad , \\
B_{40} &= -14Dq - 21D\tau \quad , \\
B_{43} &= 2\sqrt{70}\ Dq \quad .
\end{aligned}
\tag{17}
$$

Similarly for the parameters of Pryce and Runciman [13], we obtain

$$
\begin{aligned}
B_{20} &= \frac{7v - 2w}{3} \quad , \\
B_{40} &= \frac{-7Dq}{5} + \frac{2w}{3} \quad , \\
B_{43} &= -\sqrt{7/10}\left(20Dq + \frac{w}{3}\right) \quad ,
\end{aligned}
\tag{18}
$$

where $w = 2v + 3\sqrt{2}\ v'$.

In obtaining the result given in (18) we use the equations given by Macfarlane [14]. In Mcfarlane's convention, the B_{43} is negative; this has no effect on the energy levels, but introduces a phase factor in the wave function. In the tables we simply change the sign of B_{43} after it is computed by using equation (18) using values of Dq, v, and v' reported in the literature.

In all the relations given above (eq (13), (14), (17), and (18)) certain phase conventions are assumed. In order to obtain consistent values for the B_{nm}, we have frequently had to resort to changing the sign of some of the reported parameters. In some cases where theoretical levels are reported, we have resorted to fitting the theoretical results to obtain B_{nm}. Frequently, the point-charge crystal-field components, A_{nm}, indicate the correct phase relations and are used to determine the phases reported in the tables.

2.3.2 Relation between Slater and Racah parameters

For d electrons, Judd [15] gives the following relations

$$
\begin{aligned}
F_0 &= F^{(0)} \quad , \\
F_2 &= \frac{F^{(2)}}{49} \quad , \\
F_4 &= \frac{F^{(4)}}{441} \quad ,
\end{aligned}
\tag{19}
$$

and

$$E^0 = F_0 - \frac{7F_2}{2} - \frac{63F_4}{2} \quad ,$$

$$E^1 = \frac{5(F_2 + 9F_4)}{2} \quad ,$$

$$E^2 = \frac{F_2 - 5F_4}{2} \quad , \qquad (20)$$

and Racah [16] introduces A, B, and C by

$$A = F_0 - 49F_4 \quad ,$$

$$B = F_2 - 5F_4 \quad ,$$

$$C = 35F_4 \quad . \qquad (21)$$

All these parameters are used and reported in the literature. We have chosen to put all the reported data in terms of $F^{(k)}$, since Hartree-Fock calculations of $F^{(k)}$ have been reported for a large number of ions [7], and the matrix elements of the Coulomb interaction for d electrons are reported by Nielson and Koster [17] as coefficients of $F^{(k)}$. In terms of A, B, and C, we have

$$F^{(0)} = \frac{5A + 7C}{5} \quad ,$$

$$F^{(2)} = 7(7B + C) \quad , \qquad (22)$$

$$F^{(4)} = \frac{63C}{5} \quad ;$$

in terms of E^k, we have

$$F^{(0)} = E^0 - \frac{49E^1}{10} + \frac{63E^2}{2} \quad ,$$

$$F^{(2)} = \frac{49(9E^2 - E^1)}{2} \quad , \qquad (23)$$

$$F^{(4)} = \frac{441(5E^2 - E^1)}{10} \quad ,$$

and the relation between $F^{(k)}$ and F_k is given in equation (19).

2.4 Bibliographies and Reference Lists

The final section on each host material consists of a bibliography of experimental and theoretical work that has been reported. These lists, in most cases, are far from exhaustive and will be continuously updated as new work is reported or older references found. A number of hosts have only x-ray data reported, and we have been unable to find any reference to optical data on transition elements in these hosts. On a number of host materials, references were found which contain important information on that host not contained in the tables. These references have been included.

2.5 References

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3.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), of Al_2 (S_4) site for transition-metal ions with electronic configuration $3d^N$

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{44}
Sc	1	8719	-101,690	39,942
Ti	2	6819	-62,848	24,687
V	3	5606	-43,103	16,931
Cr	4	4717	-30,960	12,161
Mn	5	3999	-22,512	88,423
Fe	6	3544	-18,154	7,131
Co	7	3125	-14,396	56,545
Ni	8	2766	-11,483	4,511
Cu	9	2460	-9,228	3,625

X^{3+}	N	B_{20}	B_{40}	B_{44}
Ti	1	5057	-32,139	12,624
V	2	4251	-22,944	9,012
Cr	3	3671	-17,339	6,811
Mn	4	3212	-13,455	5,285
Fe	5	2819	-10,480	4,116
Co	6	2555	-8,796	3,455
Ni	7	2305	-7,283	2,861
Cu	8	2084	-6,054	2,378
Zn	9	1892	-50,578	1,987

X^{4+}	N	B_{20}	B_{40}	B_{44}
V	1	3951	-32,566	12,792
Cr	2	3287	-20,515	8,058
Mn	3	3121	-19,472	7,649
Fe	4	2515	-12,432	4,883
Co	5	2318	-10,239	4,022
Ni	6	2100	-8,234	3,234
Cu	7	1895	-6,523	2,562
Zn	8	1721	-5,005	1,966
Ga	9	1456	-3,252	1,277

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{44}
Sc	1	24,374	-88,055	29,364
Ti	2	19,062	-54,424	18,149
V	3	15,672	-37,325	12,447
Cr	4	13,187	-26,810	8,940
Mn	5	11,180	-19,495	6,501
Fe	6	9,906	-15,721	5,242
Co	7	8,735	-12,466	4,157
Ni	8	7,733	-6,644	3,316
Cu	9	6,877	-7,991	2,665

X^{3+}	N	B_{20}	B_{40}	B_{44}
Ti	1	14,137	-27,831	9281
V	2	11,883	-19,868	6626
Cr	3	10,261	-15,015	5007
Mn	4	8,978	-11,652	3886
Fe	5	7,881	-9,075	3026
Co	6	7,142	-7,617	2540
Ni	7	6,443	-6,307	2103
Cu	8	5,827	-5,243	1748
Zn	9	5,289	-4,380	1461

X^{4+}	N	B_{20}	B_{40}	B_{44}
V	1	11,045	-28,200	9404
Cr	2	9,188	-17,765	5924
Mn	3	8,724	-16,862	5623
Fe	4	7,031	-10,765	3590
Co	5	6,481	-8,866	2957
Ni	6	5,870	-7,131	2378
Cu	7	5,298	-5,649	1884
Zn	8	4,811	-4,334	1445
Ga	9	4,070	-2,816	939

3.3 Crystal Fields for 16(a) (C_{3i}) Site

3.3.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Al_1 (C_{3i}) site (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	6,836	-1107	-13,553	-7,823
A_{40}	-20,054	8166	3,273	-8,615
ReA_{43}	2,813	-1422	6,253	7,644
ImA_{43}	-22,370	8639	2,348	-11,383
$\|A_{43}\|$	22,546	--	--	13,711

3.5 Bibliography and References

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4. K_2NaAlF_6

4.1 Crystallographic Data on Two Forms of K_2NaAlF_6

4.1.1 Cubic T_h^6 (Pa3), 205, Z = 4, elpasoite

Ion	Site	Symmetry	x^a	y	z	q	$\alpha(Å^3)^b$
Na	4(b)	C_{3i}	1/2	1/2	1/2	1	0.147
K	8(c)	C_3	1/4	1/4	1/4	1	0.827
Al	4(a)	C_{3i}	0	0	0	3	0.0530
F	24(d)	C_1	0.22	0.03	0.01	-1	0.731

[a]X-ray data: a = 8.11 Å (reference 7).
[b]Reference 6.

4.1.2 Cubic O_h^5 (Fm3m), 225, Z = 4, elpasolite

Ion	Site	Symmetry	x^a	y	z	q	$\alpha(Å^3)^b$
Al	4(a)	O_h	0	0	0	3	0.0530
Na	4(b)	O_h	1/2	1/2	1/2	1	0.147
K	8(c)	T_d	1/4	1/4	1/4	1	0.827
F	24(e)	C_{4v}	0.219	0	0	-1	0.731

[a]X-ray data: a = 8.119 Å (reference 5).
[b]Reference 6.

4.2 Crystal Fields for Pa3 Form

4.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å$), for Al (C_{3i}) site (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Self-Induced	Dipole	Total
A_{20}	20,455	-2717	4,145	21,883
A_{40}	-15,791	8018	-10,411	-18,186
ReA_{43}	14,510	-7295	9,008	17,095
ImA_{43}	3,769	-1945	7,546	4,370

4.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for monopole A_{nm} for Al (C_{3i}) site for transition-metal ions with electronic configuration $3d^N$

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	28,077	-64,001	60,754
Ti	2	21,958	-39,556	37,550
V	3	18,053	-27,129	25,753
Cr	4	15,190	-19,486	18,498
Mn	5	12,878	-1,469	13,451
Fe	6	11,411	-11,426	10,847
Co	7	10,062	-9,061	8,601
Ni	8	8,908	-7,228	6,861
Cu	9	7,922	-5,808	5,513
X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	16,285	-20,228	19,202
V	2	13,688	-14,441	13,708
Cr	3	11,820	-10,913	10,360
Mn	4	10,343	-8,469	8,039
Fe	5	9,078	-6,596	6,261
Co	6	8,227	-5,536	5,256
Ni	7	7,422	-4,584	4,352
Cu	8	6,712	-3,810	3,617
Zn	9	6,092	-3,184	3,022
X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	12,722	-20,497	19,457
Cr	2	10,584	-12,912	12,257
Mn	3	10,050	-12,255	11,634
Fe	4	8,100	-7,824	7,428
Co	5	7,465	-6,444	6,117
Ni	6	6,761	-5,183	4,920
Cu	7	6,102	-4,106	3,897
Zn	8	5,542	-3,150	2,991
Ga	9	4,688	-2,047	1,943

K_2NaAlF_6

4.3 Crystal Fields for Fm3m Form

4.3.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Al (O_h) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{40}	23,267	15,593	-12,274	26,586
A_{44}	13,905	9,319	-7,335	15,888

$S^{(0)} = 16750\ cm^{-1}/Å^2$

$S^{(2)} = 15425\ cm^{-1}/Å^4$

$S^{(4)} = 2551.3\ cm^{-1}/Å^8$

3.3.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for Al_1 (C_{3i}) site for transition-metal ions with electronic configuration $3d^N$

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	9,379	-81,279	91,379
Ti	2	7,335	-50,235	56,478
V	3	6,031	-34,453	38,734
Cr	4	5,074	-24,747	27,822
Mn	5	4,302	-17,994	20,231
Fe	6	3,812	-14,511	16,314
Co	7	3,361	-11,507	12,937
Ni	8	2,976	-9,179	10,319
Cu	9	2,646	-7,376	8,292
X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	5440	-25,689	28,881
V	2	4573	-18,339	20,618
Cr	3	3949	-13,859	15,582
Mn	4	3455	-10,755	12,091
Fe	5	3032	-8,377	9,418
Co	6	2748	-7,031	7,905
Ni	7	2479	-5,822	6,545
Cu	8	2242	-4,839	5,440
Zn	9	2035	-4,043	4,545
X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	4250	-26,030	29,265
Cr	2	3536	-16,398	18,436
Mn	3	3357	-15,564	17,498
Fe	4	2706	-9,939	11,172
Co	5	2494	-8,184	9,201
Ni	6	2259	-6,582	7,400
Cu	7	2039	-5,214	5,862
Zn	8	1851	-4,001	4,498
Ga	9	1566	-2,599	2,922

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-10,733	-34,917	55,571
Ti	2	-8,394	-21,581	34,346
V	3	-6,902	-14,801	23,555
Cr	4	-5,807	-10,631	16,919
Mn	5	-4,923	-7,730	12,303
Fe	6	-4,362	-6,234	9,921
Co	7	-3,847	-4,943	7,867
Ni	8	-3,405	-3,943	6,276
Cu	9	-3,028	-3,169	5,043
X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-6226	-11,036	17,564
V	2	-5233	-7,878	12,539
Cr	3	-4519	-5,954	9,476
Mn	4	-3954	-4,620	7,353
Fe	5	-3470	-3,599	5,727
Co	6	-3145	-3,020	4,807
Ni	7	-2837	-2,501	3,980
Cu	8	-2566	-2,079	3,309
Zn	9	-2329	-1,739	2,764
X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-4864	-11,182	17,797
Cr	2	-4046	-7,045	11,211
Mn	3	-3842	-6,686	10,641
Fe	4	-3096	-4,269	6,794
Co	5	-2854	-3,516	5,596
Ni	6	-2585	-2,827	4,500
Cu	7	-2333	-2,240	3,565
Zn	8	-2119	-1,719	2,735
Ga	9	-1792	-1,117	1,777

$Y_3Al_5O_{12}$

3.4 Experimental Values (cm^{-1}) of B_{40}, $F^{(2)}$, and $F^{(4)}$ for nd^N Ions

Ion	B_{40}	$F^{(2)}$	$F^{(4)}$	Temp (K)	Site	Reference	nd^N
Cr^{+3}	-23,730	53,438	34,978	300	C_{3i}	1,3	$3d^3$
Cr^{+3}	-23,072	55,776	36,806	300	C_{3i}	26	$3d^3$
Cr^{+3}	-24,150	53,438	40,320	--	C_{3i}	24	$3d^3$
Cr^{+3}	35,070	--	--	--	C_{3i}	20	$3d^3$
Cr^{+3}	-22,960	54,600	40,950	77	C_{3i}	33	$3d^3$
Mn^{+3}	-27,650	59,500	32,130	300	C_{3i}	1	$3d^4$
Mn^{+4}	-27,874	53,543	43,457	300	C_{3i}	26	$3d^3$
Mn^{+4}	-29,400	--	--	--	C_{3i}	2	$3d^3$
Fe^{+3}	-26,950	39,690	15,876	300	C_{3i}	1	$3d^5$
Fe^{+3}	-17,682	49,224	36,477	--	C_{3i}	19,28	$3d^5$
Fe^{+3}	-21,756	51,023	42,979	--	S_4	19,28	$3d^5$
Fe^{+3}	-16,904	44,821	42,399	--	S_4	21	$3d^5$
Co^{+3}	-25,200	56,630	34,020	300	C_{3i}	1	$3d^6$
Co^{+3}	-17,430	--	--	--	S_4	34	$3d^6$
Co^{+2}	-9,660	--	--	--	S_4	34	$3d^7$
Co^{+2}	-12,880	--	--	--	C_{3i}	34	$3d^7$
Ni^{+3}	-27,580	42,000	22,680	300	C_{3i}	1,24	$3d^7$
Rh^{+3}	-28,840	40,600	21,924	--	C_{3i}	19	$4d^6$
Pd^{+3}	-23,730	39,326	21,218	--	C_{3i}	19	$4d^7$
Pt^{+3}	-23,100	44,520	30,744	--	C_{3i}	19	$5d^7$
V^{+3}	-23,800	--	--	--	C_{3i}	19	$3d^2$
V^{+3}	-17,850	--	--	--	S_4	19	$3d^2$
V^{+4}	-30,800	--	--	--	C_{3i}	19	$3d^1$

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3. $Y_3Al_5O_{12}$ (YAG)

3.1 Crystallographic Data on $Y_3Al_5O_{12}$

Cubic O_h^{10} (Ia3d), 230, Z = 8

Ion	Site	Symmetry	x[a]	y	z	q	α ($Å^3$)[b]
Al_1	16(a)	C_{3i}	0	0	0	3	0.0530
Al_2	24(d)	S_4	0	1/4	3/8	3	0.0530
Y	24(c)	D_2	0	1/4	1/8	3	0.870
O	96(h)	C_1	-0.0306	0.0512	0.1500	-2	1.349

[a]X-ray data: a = 12.000 Å (reference 10).
[b]Reference 23.

3.2 Crystal Fields for 24(d) (S_4) Site

3.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Al_2 (S_4) site

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	6,355	-2,604	14,013	17,765
ReA_{32}	-27,522	8,609	-11,957	-30,870
ImA_{32}	37,839	-11,913	6,332	32,258
A_{40}	-25,089	11,879	-8,516	-21,726
ReA_{44}	-3,763	1,614	1,964	-185.1
ImA_{44}	-9,108	4,740	-2,875	-7,243
ReA_{52}	-2,931	2,287	-3,498	-4,142
ImA_{52}	4,328	-3,207	3,640	4,762
$\lvert A_{44}\rvert$	9,855	--	--	7,245

4.3.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Al (O_h) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}

X^{2+}	N	B_{40}	B_{44}
Sc	1	94,301	56,357
Ti	2	58,284	34,832
V	3	39,973	23,889
Cr	4	28,711	17,159
Mn	5	20,877	12,477
Fe	6	16,836	10,062
Co	7	13,351	7,979
Ni	8	10,649	6,364
Cu	9	8,558	5,114
X^{3+}	N	B_{40}	B_{44}
Ti	1	29,805	17,812
V	2	21,278	12,716
Cr	3	16,080	9,610
Mn	4	12,478	7,457
Fe	5	9,719	5,808
Co	6	8,157	4,875
Ni	7	6,754	4,037
Cu	8	5,614	3,355
Zn	9	4,691	2,803
X^{4+}	N	B_{40}	B_{44}
V	1	30,201	18,049
Cr	2	19,025	11,370
Mn	3	18,058	10,792
Fe	4	11,529	6,890
Co	5	9,495	5,675
Ni	6	7,636	4,564
Cu	7	6,049	3,615
Zn	8	4,642	2,774
Ga	9	3,015	1,802

(b) For total A_{nm}

X^{2+}	N	B_{40}	B_{44}
Sc	1	107,750	64,394
Ti	2	66,598	39,799
V	3	45,675	27,296
Cr	4	32,807	19,606
Mn	5	23,856	14,256
Fe	6	19,238	11,497
Co	7	15,255	9,117
Ni	8	12,168	7,272
Cu	9	9,778	5,844
X^{3+}	N	B_{40}	B_{44}
Ti	1	34,057	20,353
V	2	24,313	14,530
Cr	3	18,374	10,980
Mn	4	14,258	8,521
Fe	5	11,105	6,636
Co	6	9,321	5,570
Ni	7	7,718	4,612
Cu	8	6,415	3,834
Zn	9	5,360	3,203
X^{4+}	N	B_{40}	B_{44}
V	1	34,509	20,623
Cr	2	21,739	12,992
Mn	3	20,633	12,331
Fe	4	13,173	7,873
Co	5	10,850	6,484
Ni	6	87,255	5,214
Cu	7	6,912	4,131
Zn	8	5,304	3,170
Ga	9	3,446	2,059

K_2NaAlF_6

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5. Cs_2TiF_6

5.1 Crystallographic Data on Two Forms of Cs_2TiF_6

5.1.1 Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)^b
Ti	4(a)	O_h	0	0	0	+4	0.506
Cs	8(c)	T_d	1/4	1/4	1/4	+1	2.492
F	24(e)	C_{4v}	0.195	0	0	−1	0.731

[a]X-ray data: a = 8.96 Å; the F position is not reported for Cs_2TiF_6 and is taken from Cs_2MnF_6 (reference 3, p 341).
[b]Reference 2.

5.1.2 Hexagonal D_{3d}^3 ($P\bar{3}m1$), 164, Z = 1

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)^b
Ti	1(a)	D_{3d}	0	0	0	+4	0.506
Cs	2(d)	C_{3v}	1/3	2/3	0.691	+1	2.492
F	6(i)	C_s	0.167	−0.167	0.206	−1	0.731

[a]X-ray data, a = 6.15 Å, c = 4.96 Å; the Cs and F positions are not reported for Cs_2TiF_6 and are taken from Cs_2ZrF_6 (reference 3, p 350).
[b]Reference 2.

5.2 Crystal Fields for O_h Site

5.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Ti (O_h) site of cubic form

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{40}	25,400	32,148	−14,102	43,445
A_{44}	15,179	19,212	−8,428	25,963

$S^{(0)} = 18,682\ cm^{-1}/Å^2$

$S^{(2)} = 17,743\ cm^{-1}/Å^4$

$S^{(4)} = 3148.1\ cm^{-1}/Å^8$

Cs_2TiF_6

5.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Ti (O_h) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}

X^{2+}	N	B_{40}	B_{44}
Sc	1	102,950	61,520
Ti	2	63,627	38,023
V	3	43,637	26,078
Cr	4	31,344	18,731
Mn	5	22,791	13,620
Fe	6	18,379	10,984
Co	7	14,575	8,710
Ni	8	11,626	6,947
Cu	9	9,342	5,583
X^{3+}	N	B_{40}	B_{44}
Ti	1	32,537	19,444
V	2	23,228	13,881
Cr	3	17,554	10,490
Mn	4	13,622	8,141
Fe	5	10,610	6,340
Co	6	8,905	5,322
Ni	7	7,374	4,407
Cu	8	6,129	3,663
Zn	9	5,121	3,060
X^{4+}	N	B_{40}	B_{44}
V	1	32,969	19,702
Cr	2	20,770	12,412
Mn	3	19,713	11,780
Fe	4	12,586	7,521
Co	5	10,366	6,195
Ni	6	8,366	4,982
Cu	7	6,604	3,947
Zn	8	5,067	3,028
Ga	9	3,292	1,967

(b) For total A_{nm}

X^{2+}	N	B_{40}	B_{44}
Sc	1	176,080	105,230
Ti	2	108,830	65,037
V	3	74,639	44,604
Cr	4	53,611	3,2038
Mn	5	38,983	23,297
Fe	6	31,437	18,787
Co	7	24,929	14,898
Ni	8	19,885	11,883
Cu	9	15,979	9,549
X^{3+}	N	B_{40}	B_{44}
Ti	1	55,653	33,259
V	2	39,730	23,743
Cr	3	30,025	17,943
Mn	4	23,300	13,924
Fe	5	18,147	10,845
Co	6	15,232	9,103
Ni	7	12,612	7,537
Cu	8	10,483	6,265
Zn	9	8,759	5,234
X^{4+}	N	B_{40}	B_{44}
V	1	56,392	33,700
Cr	2	35,525	21,230
Mn	3	33,718	20,150
Fe	4	21,527	12,865
Co	5	17,730	10,596
Ni	6	14,259	8,521
Cu	7	11,296	6,750
Zn	8	8,667	5,180
Ga	9	5,631	3,365

5.3 Crystal Fields for D_{3d} Site

5.3.1 Crystal-field components, A_{nm} (cm^{-1}/Å), for Ti (D_{3d}) site in hexagonal form

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	-5629	-3291	1172	-7748
A_{40}	-5090	-3546	1986	-6651
A_{43}	10051	6316	-3059	13308

$S^{(0)} = 8919.9\ cm^{-1}/Å^2$

$S^{(2)} = 5251.8\ cm^{-1}/Å^4$

$S^{(4)} = 460.86\ cm^{-1}/Å^8$

5.3.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Ti (D_{3d}) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-7723	-20,630	40,737
Ti	2	-6040	-12,750	25,178
V	3	-4966	-8,745	17,268
Cr	4	-4178	-6,281	12,403
Mn	5	-3542	-4,567	9,019
Fe	6	-3139	-3,683	7,273
Co	7	-2768	-2,921	5,767
Ni	8	-2450	-2,330	4,600
Cu	9	-2179	-1,872	3,697

X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-4480	-6520	12,875
V	2	-3765	-4655	9,192
Cr	3	-3251	-3518	6,946
Mn	4	-2845	-2730	5,390
Fe	5	-2497	-2126	4,198
Co	6	-2263	-1785	3,524
Ni	7	-2042	-1478	2,918
Cu	8	-1846	-1228	2,425
Zn	9	-1676	-1026	2,026

X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-3500	-6607	13,046
Cr	2	-2911	-4162	8,219
Mn	3	-2764	-3950	7,801
Fe	4	-2228	-2522	4,980
Co	5	-2054	-2077	4,102
Ni	6	-1860	-1671	3,299
Cu	7	-1679	-1323	2,613
Zn	8	-1524	-1016	2,005
Ga	9	-1290	-660	1,303

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
SC	1	-10,630	-26,957	53,937
Ti	2	-8,314	-16,661	33,337
V	3	-6,835	-11,426	22,863
Cr	4	-5,751	-8,207	16,422
Mn	5	-4,876	-5,968	11,941
Fe	6	-4,320	-4,813	9,630
Co	7	-3,810	-3,816	7,636
Ni	8	-3,373	-3,044	6,091
Cu	9	-2,999	-2,446	4,895

X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-6166	-8520	17,048
V	2	-5183	-6082	12,170
Cr	3	-4475	-4597	9,197
Mn	4	-3916	-3567	7,137
Fe	5	-3437	-2778	5,559
Co	6	-3115	-2332	4,666
Ni	7	-2810	-1931	3,863
Cu	8	-2541	-1605	3,211
Zn	9	-2307	-1341	2,683

X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-4817	-8633	17,274
Cr	2	-4007	-5439	10,882
Mn	3	-3805	-5162	10,328
Fe	4	-3067	-3296	6,594
Co	5	-2827	-2714	5,431
Ni	6	-2560	-2183	4,368
Cu	7	-2311	-1729	3,460
Zn	8	-2098	-1327	2,655
Ga	9	-1775	-862	1,725

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6. $NH_4Al(SO_4)_2$

6.1 Crystallographic Data on $NH_4Al(SO_4)_2$

Trigonal D_3^2 (P321) (hexagonal setting), 150, Z = 1

Ion	Site	Symmetry	x[a]	y	z	q	α ($Å^3$)[b]
NH_4	1(a)	D_3	0	0	0	1	2.684
Al	1(b)	D_3	0	0	1/2	3	0.0530
S	2(d)	C_3	1/3	2/3	0.222	6	4.893
O_1	2(d)	C_3	1/3	2/3	0.016	-2	1.349
O_2	6(g)	C_2	0.328	0.344	0.317	-2	1.349

[a]X-ray data: a = 4.724 Å, c = 8.225 Å; the positions for S, O_1, and O_2 in $NH_4Al(SO_4)_2$ are not given. Those listed above are for the same ions in $KAl(SO_4)_2$ (reference 3).
[b]Reference 2.

6.2 Crystal Fields for Al (D_2) Site

6.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$) for Al (D_2) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	13,668	-42,591	-2720.0	-41,994.49
A_{33}	10,708	-17,390	-1961.9	--
A_{40}	-4,089.1	25,994	4005.7	25,293.63
A_{43}	8,105.7	-36,041	840.80	3,661.09
A_{53}	5,996.4	-15,968	-2489.0	--

$S^{(0)} = 15{,}593\ cm^{-1}/Å^2$
$S^{(2)} = 7176.6\ cm^{-1}/Å^4$
$S^{(4)} = 444.17\ cm^{-1}/Å^8$

6.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Al (D_2) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm} / **(b) For total A_{nm}**

X^{2+}	N	B_{20}	B_{40}	B_{43}	X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	18,752	-16,573	32,852	Sc	1	-57,616	102,520	14,838
Ti	2	14,666	10,243	20,305	Ti	2	-45,060	63,361	9,171
V	3	12,058	-7,025	13,926	V	3	-37,048	43,454	6,290
Cr	4	10,146	-5,046	10,002	Cr	4	-31,173	31,212	4,518
Mn	5	8,601	-3,669	7,273	Mn	5	-26,427	22,696	3,285
Fe	6	7,621	-2,959	5,865	Fe	6	-23,416	18,302	2,649
Co	7	6,721	-2,346	4,651	Co	7	-20,649	14,513	2,101
Ni	8	5,950	-1,872	3,710	Ni	8	-18,280	11,577	1,676
Cu	9	5,291	-1,504	2,981	Cu	9	-16,256	9,303	1,347
X^{3+}	N	B_{20}	B_{40}	B_{43}	X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	10,877	-5238	10,383	Ti	1	-33,419	32,401	4690
V	2	9,143	-3740	7,413	V	2	-28,090	23,131	3348
Cr	3	7,895	-2826	5,602	Cr	3	-24,256	17,480	2530
Mn	4	6,908	-2193	4,347	Mn	4	-21,224	13,565	1963
Fe	5	6,063	-1708	3,386	Fe	5	-18,629	10,565	1529
Co	6	5,495	-1434	2,842	Co	6	-16,882	8,868	1284
Ni	7	4,957	-1187	2,353	Ni	7	-15,231	7,343	1063
Cu	8	4,483	-987	1,956	Cu	8	-13,774	6,103	883
Zn	9	4,069	-824	1,634	Zn	9	-12,502	5,099	738
X^{4+}	N	B_{20}	B_{40}	B_{43}	X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	8497	-5308	10,521	V	1	-26,108	32,831	4752
Cr	2	7069	-3344	6,628	Cr	2	-21,720	20,683	2994
Mn	3	6712	-3174	6,291	Mn	3	-20,623	19,630	2841
Fe	4	5410	-2026	4,016	Fe	4	-16,621	12,533	1814
Co	5	4986	-1669	3,308	Co	5	-15,320	10,322	1494
Ni	6	4516	-1342	2,660	Ni	6	-13,875	8,301	1202
Cu	7	4076	-1063	2,108	Cu	7	-12,523	6,576	952
Zn	8	3701	-816	1,617	Zn	8	-11,372	5,046	730
Ga	9	3131	-530	1,051	Ga	9	-9,621	3,278	474

6.3 Experimental Parameters (cm^{-1})

Ion	$F^{(2)}$	$F^{(4)}$	ζ	α	B_{40}	Reference
Cr^{3+}	--	--	186	--	-38,156	1

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7. MgF_2

7.1 Crystallographic Data on MgF_2

Tetragonal D_{4h}^{14} ($P4_2/mnm$), 136, Z = 2

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)^b
Mg	2(a)	D_{2h}	0	0	0	+2	0.0809
F	4(f)	C_{2v}	0.303	0.303	0	−1	0.731

[a]X-ray data: a = 4.623 Å, c = 3.052 Å (reference 16).
[b]Reference 12.

7.2 Crystal Fields for Mg (D_{2h}) Site

7.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Mg (D_{2h}) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	−576.3	3745	−592.7	2576
A_{22}	2,447	−1807	−327.8	312.6
A_{40}	−3,020	−381.7	660.3	−2742
A_{42}	−10,015	−212.2	3965	−6262
A_{44}	4,458	−513.4	−2057	1887

$S^{(0)} = 8871\ cm^{-1}/Å^2$
$S^{(2)} = 6315\ cm^{-1}/Å^4$
$S^{(4)} = 656.0\ cm^{-1}/Å^8$

7.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Mg (D_{2h}) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Sc	1	-791	3357	-12,240	-40,591	18,068
Ti	2	-618	2626	-7,565	-25,088	11,167
V	3	-508	2159	-5,188	-17,206	76,59
Cr	4	-428	1816	-3,727	-12,359	5,501
Mn	5	-363	1540	-2,710	-8,987	4,000
Fe	6	-321	1364	-2,185	-7,247	3,226
Co	7	-283	1203	-1,733	-5,747	2,558
Ni	8	-251	1065	-1,382	-4,584	2,040
Cu	9	-223	947	-1,111	-3,684	1,640

X^{3+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{40}
Ti	1	-459	1947	-3867	-12,829	5711
V	2	-385	1637	-2762	-9,159	4077
Cr	3	-333	1413	-2087	-6,921	3081
Mn	4	-291	1237	-1620	-5,371	2391
Fe	5	-256	1086	-1262	-4,183	1862
Co	6	-232	984	-1059	-3,511	1563
Ni	7	-209	888	-877	2,907	1294
Cu	8	-189	803	-729	-2,417	1076
Zn	9	-172	728	-609	-2,019	899

X^{4+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
V	1	-358	1521	-3920	-12,999	5787
Cr	2	-298	1266	-2470	-8,189	3645
Mn	3	-283	1202	-2344	-7,773	3460
Fe	4	-228	969	-1496	-4,962	2209
Co	5	-210	893	-1233	-4,087	1819
Ni	6	-190	808	-991	-3,287	1463
Cu	7	-172	730	-785	-2,604	1159
Zn	8	-156	663	-602	-1,998	889
Ga	9	-132	561	-391	-1,298	578

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Sc	1	3534	429	-11,113	-25,380	7648
Ti	2	2764.	335	-6,869	-15,686	4727
V	3	2273	276	-4,711	-10,758	3242
Cr	4	1912	232	-3,384	-7,727	2329
Mn	5	1621	197	-2,460	-5,619	1693
Fe	6	1436	174	-1,984	-4,531	1365
Co	7	1267	154	-1,573	-3,593	1083
Ni	8	1121	136	-1,255	-2,866	864
Cu	9	997	121	-1,009	-2,303	694

X^{3+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Ti	1	2050	249	-3513	-8022	2417
V	2	1723	209	-2508	-5727	1726
Cr	3	1488	181	-1895	-4328	1304
Mn	4	1302	158	-1471	-3358	1012
Fe	5	1143	139	-1145	-2616	788
Co	6	1036	126	-961	-2196	662
Ni	7	934	113	-796	-1818	548
Cu	8	845	103	-662	-1511	455
Zn	9	767	93	-553	-1262	380

X^{4+}	N	B_{20}	B_{22}	B_{40}	B_{44}	B_{44}
V	1	1602	194	-3559	-8128	2449
Cr	2	1332	162	-2242	-5120	1543
Mn	3	1265	154	-2128	-4860	1465
Fe	4	1020	124	-1359	-3103	935
Co	5	940	114	-1119	-2556	770
Ni	6	851	103	-900	-2055	619
Cu	7	768	93	-713	-1628	491
Zn	8	698	85	-547	-1249	376
Ga	9	590	72	-355	-812	245

7.3 Experimental Parameters (cm^{-1})

Ion	$F^{(2)}$	$F^{(4)}$	α	ζ	B_{40}[a]	Reference
V^{2+}	53,362	28,065	79	--	24,150	10
V^{2+}	49,508	34,871	--	--	21,735	19

[a]Cubic approximation $B_{44} = \sqrt{5/14}\,|B_{40}|$

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8. MnF_2

8.1 Crystallographic Data on MnF_2

Tetragonal D_{4h}^{14} ($P4_2/mnm$), 136, Z = 2

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)[b]
Mn	2(a)	D_{2h}	0	0	0	+2	0.122
F	4(f)	C_{2v}	0.305	0.305	0	-1	0.731

[a]X-ray data: a = 4.8734 Å, c = 3.3099 Å (reference 18).
[b]Reference 14.

8.2 Crystal Fields for Mn (D_{2h}) Site

8.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Mn (D_{2h}) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	901.5	1815.67	-459.22	2258
A_{22}	2638	-847.40	-300.87	1490
A_{40}	-1670	-125.49	266.58	-1529
A_{42}	-7263	-61.74	2376.30	-4948
A_{44}	3218	-222.98	-1239.99	1755

$S^{(0)} = 6,070\ cm^{-1}/Å^2$
$S^{(2)} = 3,813\ cm^{-1}/Å^4$
$S^{(4)} = 307.3\ cm^{-1}/Å^8$

8.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Mn (D_{2h}) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}"

X^{2+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Sc	1	1237	3619	-6769	-29,437	13,043
Ti	2	967	2831	-4183	-18,194	8,061
V	3	795	2327	-2869	-12,478	5,529
Cr	4	669	1958	-2061	-8,963	3,971
Mn	5	567	1660	-1499	-6,517	2,888
Fe	6	503	1471	-1208	-5,256	2,329
Co	7	443	1297	-958	-4,168	1,847
Ni	8	392	1148	-764	-3,324	1,473
Cu	9	349	1021	-614	-2,671	1,184

X^{3+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Ti	1	717	2099	-2139	-9304	4122
V	2	603	1765	-1527	-6642	2943
Cr	3	521	1524	-1154	-5020	2224
Mn	4	456	1333	-896	-3895	1726
Fe	5	400	1170	-698	-3034	1344
Co	6	362	1061	-586	-2546	1128
Ni	7	327	957	-485	-2108	934
Cu	8	296	865	-403	-1753	777
Zn	9	268	785	-337	-1464	649

X^{4+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
V	1	560	1640	-2168	-9427	4177
Cr	2	466	1364	-1366	-5939	2631
Mn	3	443	1296	-1296	-5637	2498
Fe	4	357	1044	-827	-3599	1595
Co	5	329	962	-682	-2964	1313
Ni	6	298	872	-548	-2384	1056
Cu	7	269	787	-434	-1888	837
Zn	8	244	714	-333	-1449	642
Ga	9	207	604	-216	-941	417

MnF_2

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Sc	1	3098	2044	-6197	-20,054	7113
Ti	2	2423	1599	-3830	-12,395	4396
V	3	1992	1315	-2627	-8,501	3015
Cr	4	1676	1106	-1887	-6,106	2166
Mn	5	1421	938	-1372	-4,440	1575
Fe	6	1259	831	-1106	-3,580	1270
Co	7	1110	733	-877	-2,839	1007
Ni	8	983	649	-700	-2,265	803
Cu	9	874	577	-562	-1,820	645

X^{3+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Ti	1	1797	1186	-1959	-6338	2248
V	2	1510	997	-1398	-4525	1605
Cr	3	1304	861	-1057	-3420	1213
Mn	4	1141	753	-820	-2654	941
Fe	5	1002	661	-639	-2067	733
Co	6	908	599	-536	-1735	615
Ni	7	819	540	-444	-1436	509
Cu	8	741	489	-369	-1194	423
Zn	9	672	444	-308	-998	354

X^{4+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
V	1	1404	926	-1985	-6423	2278
Cr	2	1168	771	-1250	-4046	1435
Mn	3	1109	732	-1187	-3840	1362
Fe	4	894	590	-758	-2452	870
Co	5	824	544	-624	-2019	716
Ni	6	746	492	-502	-1624	576
Cu	7	673	444	-398	-1287	456
Zn	8	611	403	-305	-987	350
Ga	9	517	341	-198	-641	227

8.3 Experimental Parameters (cm^{-1})

Ion	$F^{(2)}$	$F^{(4)}$	α	ζ	B_{40}[a]	Reference
Co^{2+}	--	--	--	--	17,220	2
Mn^{2+}	62,230	39,690	76	320	15,750	10
Mn^{2+}	61,355	39,791	76	320	15,792	10
Mn^{2+}	58,849	46,746	--	--	17,220	4
Mn^{2+}	67,830	41,215	66.1	--	16,569	15
Mn^{2+}	67,550	41,240	65	--	17,300	19[b]
Mn^{2+}	69,510	41,328	--	--	16,380	16

[a]Cubic approximation $B_{44} = \sqrt{5/14}\ B_{40}$

[b]Fit with full D_{2h} symmetry; $B_{20} = -1480$, $B_{22} = 4750$, $B_{42} = -1650$, $B_{44} = -10{,}260$.

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9. ZnF_2

9.1 Crystallographic Data on ZnF_2

Tetragonal D_{4h}^{14} ($P4_2/mnm$), 136, Z = 2

Ion	Site	Symmetry	x[a]	y	z	q	α (Å³)[b]
Zn	2(a)	D_{2h}	0	0	0	+2	0.676
F	4(f)	C_{2v}	0.303	0.303	0	−1	0.731

[a]X-ray data: a = 4.7034 Å, c = 3.1335 Å (reference 10); a, c same, but x_F = 0.307 (reference 8).
[b]Reference 7.

9.2 Crystal Fields for Zn Site (D_{2h})

9.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Zn (D_{2h}) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	-304.8	2855	-593.0	1957
A_{22}	2659	-1379	-346.0	934.0
A_{40}	-249.1	-268.3	430.1	-2329
A_{42}	-9011	-135.5	3350	-5796
A_{44}	-4046	-383.2	1786	-1876

$S^{(0)} = 8214.0\ cm^{-1}/Å^2$

$S^{(2)} = 5417.7\ cm^{-1}/Å^4$

$S^{(4)} = 508.50\ cm^{-1}/Å^8$

9.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Zn (D_{2h}) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Sc	1	-418	3648	-1010	-36,522	-16,398
Ti	2	-327	2853	-624	-22,573	-10,135
V	3	-269	2346	-428	-15,481	-6,951
Cr	4	-226	1974	-307	-11,120	-4,993
Mn	5	-192	1673	-224	-8,086	-3,631
Fe	6	-170	1483	-180	-6,520	-2,928
Co	7	-150	1307	-143	-5,171	-2,322
Ni	8	-133	1158	-114	-4,124	-1,852
Cu	9	-118	1029	-92	-3,314	-1,488
X^{3+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Ti	1	-243	2116	-319	-11,543	-5183
V	2	-204	1779	-228	-8,241	-3700
Cr	3	-176	1536	-172	-6,228	-2796
Mn	4	-154	1344	-134	-4,833	-2170
Fe	5	-135	1180	-104	-3,764	-1690
Co	6	-123	1069	-87	-3,159	-1419
Ni	7	-11	964	-72	-2,616	-1175
Cu	8	-100	872	-60	-2,174	-976
Zn	9	-91	792	-50	-1,817	-816
X^{4+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
V	1	-189	1653	-323	-11,696	-5252
Cr	2	-158	1375	-204	-7,368	-3308
Mn	3	-150	1306	-193	-6,993	-3140
Fe	4	-121	1052	-123	-4,465	-2005
Co	5	-111	970	-102	-3,677	-1651
Ni	6	-101	879	-82	-2,957	-1328
Cu	7	-91	793	-65	-2,343	-1052
Zn	8	-83	720	-50	-1,798	-807
Ga	9	-70	609	-32	-1,168	-524

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Sc	1	2685	1281	-9439	-23,491	-7603
Ti	2	2100	1002	-5834	-14,519	-4699
V	3	1727	824	-4001	-9,958	-3223
Cr	4	1453	693	-2874	-7,152	-2315
Mn	5	1232	588	-2090	-5,201	-1683
Fe	6	1091	521	-1685	-4,194	-1358
Co	7	962	459	-1336	-3,326	-1076
Ni	8	852	407	-1066	-2,653	-859
Cu	9	758	362	-857	-2,132	-690

X^{3+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
Ti	1	1557	743	-2983	-7425	-2403
V	2	1309	625	-2130	-5300	-1716
Cr	3	1130	539	-1610	-4006	-1297
Mn	4	989	472	-1249	-3108	-1006
Fe	5	868	414	-973	-2421	-784
Co	6	787	375	-817	-2032	-658
Ni	7	710	339	-676	-1683	-545
Cu	8	642	306	-562	-1399	-453
Zn	9	583	278	-470	-1169	-378

X^{4+}	N	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}
V	1	1217	581	-3023	-7523	-2435
Cr	2	1012	483	-1904	-4739	-1534
Mn	3	961	459	-1808	-4498	-1456
Fe	4	775	370	-1154	-2872	-930
Co	5	714	341	-950	-2365	-766
Ni	6	647	309	-764	-1902	-616
Cu	7	584	279	-606	-1507	-488
Zn	8	530	253	-465	-1156	-374
Ga	9	448	214	-302	-751	-243

9.3 Experimental Parameters (cm^{-1})

Ion	$F^{(2)}$	$F^{(4)}$	α	β	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}	Ref
Mn^{2+}	57,550	41,240	65	337	-920	3730	21,180	-1390	-12,660	11

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10. MgO

10.1 Crystallographic Data on MgO

Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)^b
Mg	4(a)	O_h	0	0	0	+2	0.0809
O	4(b)	O_h	1/2	1/2	1/2	-2	1.349

[a]X-ray data, a = 4.2112 (reference 54).
[b]Reference 45.

10.2 Crystal Fields for Mg (O_h) Site

10.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Mg (O_h) site

A_{nm}	Monopole	Self-induced	Total
A_{40}	20,084	-5,812	14,271
A_{44}	12,002	-3,474	8,528.8

$S^{(0)}$ = 11,851 $cm^{-1}/Å^2$
$S^{(2)}$ = 7523.7 $cm^{-1}/Å^4$
$S^{(4)}$ = 621.35 $cm^{-1}/Å^8$

10.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of $Mg_N(O_h)$ site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}				(b) For total A_{nm}			
X^{2+}	N	B_{40}	B_{44}	X^{2+}	N	B_{40}	B_{44}
Sc	1	81,400	48,644	Sc	1	57,840	34,567
Ti	2	50,310	30,065	Ti	2	35,749	21,365
V	3	34,504	20,619	V	3	24,518	14,652
Cr	4	24,784	14,810	Cr	4	17,610	10,525
Mn	5	18,021	10,769	Mn	5	12,805	7,653
Fe	6	14,533	8,685	Fe	6	10,326	6,171
Co	7	11,[illegible]24	6,887	Co	7	8,188	4,894
Ni	8	9,19[illegible]	5,493	Ni	8	6,532	3,904
Cu	9	7,387	4,414	Cu	9	5,249	3,137
X^{3+}	N	B_{40}	B_{44}	X^{3+}	N	B_{40}	B_{44}
Ti	1	25,728	15,375	Ti	1	18,281	10,925
V	2	18,367	10,976	V	2	13,051	7,800
Cr	3	13,880	8,295	Cr	3	9,863	5,894
Mn	4	10,771	6,437	Mn	4	7,654	4,574
Fe	5	8,389	5,013	Fe	5	5,961	3,563
Co	6	7,042	4,208	Co	6	5,003	2,990
Ni	7	5,830	3,484	Ni	7	4,143	2,476
Cu	8	4,846	2,896	Cu	8	3,444	2,058
Zn	9	4,049	2,420	Zn	9	2,877	1,719
X^{4+}	N	B_{40}	B_{44}	X^{4+}	N	B_{40}	B_{44}
V	1	26,069	15,579	V	1	18,524	11,070
Cr	2	16,423	9,814	Cr2	2	11,669	6,974
Mn	3	15,587	9,315	Mn	3	11,076	6,619
Fe	4	9,952	5,947	Fe4	4	7,071	4,226
Co	5	8,196	4,898	Co	5	5,824	3,481
Ni	6	6,592	3,939	Ni6	6	4,684	2,799
Cu	7	5,222	3,121	Cu	7	3,711	2,218
Zn	8	4,007	2,394	Zn	8	2,847	1,702
Ga	9	2,603	1,556	Ga	9	1,850	1,105

10.3 Experimental Parameters (cm^{-1})

Ion	$F^{(2)}$	$F^{(4)}$	α	B_{40}	Ref.
Cr^{3+}	50,906	37,825	70	33,579	52
V^{2+}	42,429	30,239	60	30,429	52
V^{2+}	47,625	25,455	79	29,400	48
Cr^{3+}	52,780	36,792	70	33,390	7[a]
Cr^{3+}	54,600	40,950	--	34,020	25[b]
Cr^{3+}	54,250	40,320	--	34,860	32[c]
Cr^{2+}	--	--	--	14,000	12
Ni^{2+}	--	--	--	18,060	27[d]
Ni^{2+}	--	--	--	17,115	40
Ni^{2+}	66,343	44,447	--	17.451	37[e]

[a] $\zeta = 270$

[b] $\zeta = 135$

[c] $\zeta = 210$

[d] Refers to experimental optical data by A. G. Shenstone (reference 46).

[e] $\zeta = 645$

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11. $Be_3Al_2(SiO_3)_6$ (Beryl, Emerald)

11.1 Crystallographic and X-Ray Data on $Be_3Al_2(SiO_3)_6$

Hexagonal D_{6h}^2 (P6/mcc), 192, Z = 2

Ion	Site	Symmetry	x[a]	y	z	q	$\alpha(Å)^3$[b]
Al	4(c)	D_3	1/3	2/3	1/4	+3	0.0530
Be	6(f)	D_2	1/4	0	1/4	+2	0.0125
Si	12(ℓ)	C_s	0.382	0.118	0	+4	0.0165
O_1	12(ℓ)	C_s	0.294	0.242	0	-2	1.349
O_2	24(m)	C_1	0.499	0.143	0.138	-2	1.349

[a]X-ray data: a = 9.206 Å, c = 9.205 Å (reference 14).
[b]Reference 9.

11.2 Crystal Fields for Al (D_3) Site

11.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Al (D_3) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	-16,578	13,630	1289	-1659
A_{33}	-i14,113	-i2,941	i2339	-i14716
A_{40}	-16,436	-23,937	6117	-34257
A_{43}	20,357	29,273	-8341	41288
A_{53}	-i14,004	-i3,056	i1543	-i5516

$S^{(0)} = 18,026\ cm^{-1}/Å^2$

$S^{(2)} = 13,560\ cm^{-1}/Å^4$

$S^{(4)} = 1,535.7\ cm^{-1}/Å^8$

11.2.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for A_{nm} of Al (D_3) site for transition-metal ions with electronic configuration nd^N

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-22,745	-66,615	82,507
Ti	2	-17,788	-41,172	50,994
V	3	-14,625	-28,237	34,973
Cr	4	-12,306	-20,282	25,121
Mn	5	-10,433	-14,748	18,266
Fe	6	-9,244	-11,893	14,730
Co	7	-8,151	-9,431	11,681
Ni	8	-7,216	-7,523	9,317
Cu	9	-6,417	-6,045	7,487
X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-13,193	-21,055	26,077
V	5	-11,089	-15,031	18,616
Cr	3	-9,576	-11,359	14,069
Mn	4	-8,379	-8,815	10,917
Fe	5	-7,354	-6,865	8,503
Co	6	-6,664	-5,763	7,137
Ni	7	-6,013	-4,771	5,910
Cu	8	-5,438	-3,966	4,912
Zn	9	-4,935	-3,314	4,104
X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-10,307	-21,334	26,423
Cr	2	-8,574	-13,440	16,646
Mn	3	-8,142	-12,756	15,799
Fe	4	-6,562	-8,144	10,087
Co	5	-6,048	-6,708	8,308
Ni	6	-5,477	-5,394	6,681
Cu	7	-4,944	-4,273	5,293
Zn	8	-4,489	-3,279	4,061
Ga	9	-3,798	-2,130	2,638

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-2276	-138,840	167,340
Ti	2	-1780	-85,814	103,430
V	3	-1464	-58,854	70,933
Cr	4	-1232	-42,273	50,949
Mn	5	-1044	-30,739	37,048
Fe	6	-925	-24,788	29,876
Co	7	-816	-19,657	23,691
Ni	8	-722	-15,679	18,898
Cu	9	-642	-12,600	15,186
X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-1320	-43,883	52,890
V	2	-1110	-31,328	37,758
Cr	3	-958	-23,675	28,534
Mn	4	-838	-18,372	22,143
Fe	5	-736	-14,309	17,246
Co	6	-667	-12,011	14,476
Ni	7	-602	-9,945	11,986
Cu	8	-544	-8,266	9,963
Zn	9	-494	-6,906	8,324
X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-1031	-44,466	53,592
Cr	2	-858	-28,012	33,761
Mn	3	-815	-26,587	32,044
Fe	4	-657	-16,974	20,458
Co	5	-605	-13,980	16,850
Ni	6	-548	-11,243	13,551
Cu	7	-495	-8,907	10,735
Zn	8	-449	-6,834	8,237
Ga	9	-380	-4,440	5,351

11.3 Experimental Parameters (cm^{-1})

Ion	$F^{(2)}$	$F^{(4)}$	α	ζ	B_{20}	B_{40}	B_{43}	Ref
Cr^{3+}	58,940	37,296	--	--	--	-2,280	2,725.12	5
V^{3+}	49,560	37,170	--	--	-2742	-24,652	27,187	3

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12. $Na_3M_2Li_3F_{12}$ (Fluoride Garnets)

12.1 Crystallographic Data on $Na_3M_2Li_3F_{12}$

Cubic O_h^{10} (Ia3d), 230, Z = 8

Ion	Site	Symmetry	x	y	z	q	α ($Å^3$)
M	16(a)	C_{3i}	0	0	0	3	α_x
Na	24(e)	D_2	0	1/4	1/8	1	0.147[a]
Li	24(d)	S_4	0	1/4	3/8	1	0.0321[a]
F	96(f)	C_1	x	y	z	-1	0.731[a]

[a]Reference 18.

12.2 X-Ray Data on $Na_3M_2Li_3F_{12}$

M	a (Å)	x	y	z	α_x ($Å^3$)	Ref.
Al	12.122	-0.02888	0.04268	0.13989	0.0530	21
Sc	12.607	-0.0343	0.0499	0.1407	0.0540	14
In	12.693	-0.0349	0.0507	0.1422	0.574	14
Ti	12.498	-0.035	0.050	0.140	0.33[a]	13
V	12.409	-0.035	0.050	0.140	0.31[a]	13
Cr	12.328	-0.035	0.050	0.140	0.29[a]	13
Mn	12.141	--	--	--	0.27[a]	--
Fe	12.393	-0.035	0.050	0.140	0.24[a]	13
Fe	12.387	-0.02954	0.04737	0.14538	0.24[a]	10
Co	12.326	-0.035	0.050	0.140	0.23[a]	13
Ni	12.446	--	--	--	0.22[a]	--
Rh	12.415	-0.035	0.050	0.140	0.71[a]	13

[a]Reference 6.

12.3 Crystal-Field Data

12.3.1 Crystal-field components, A_{nm} (cm /Å^n), for M (C_{3i}) site in $Na_3M_2Li_3F_{12}$ (rotated so that z-axis is along (111) crystallographic axis)

M	Monopole			Total		
	A_{20}	A_{40}	A_{43}	A_{20}	A_{40}	A_{43}
Al	-2051	-14,470	16,491	732.8	-15,454	18,471
Sc	107.7	-10,058	11,840	-307.3	-11,064	13,385
In	-123.3	-9,150	10,803	-482.5	-10,065	12,202
Ti	-466.9	-10,590	12,596	-841.2	-11,667	14,241
V	-477.0	-10,975	13,054	-881.1	-12,090	14,770
Cr	-486.5	-11,340	13,489	-919.6	-12,492	15,273
Fe	-478.8	-11,046	13,139	-888.6	-12,168	14,868
Fe	-3026	-10,404	11,650	1966.2	-11,351	13,247
Co	-486.7	-11,349	13,500	-920.6	-12,502	15,285
Rh	-476.3	-10,948	13,023	-878.4	-12,062	14,734

12.3.2 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for Al (C_{3i}) site of $Na_3Al_2Li_3F_{12}$ for transition-metal ions with electronic configuration $3d^N$

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-2814	-58,646	66,838
Ti	2	-2201	-36,247	41,310
V	3	-1809	-24,859	28,332
Cr	4	-1522	-17,856	20,350
Mn	5	-1291	-12,984	14,797
Fe	6	-1144	-10,470	11,933
Co	7	-1008	-8,303	9,463
Ni	8	-893	-6,623	7,548
Cu	9	-794	-5,322	6,065

X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-1632	-18,536	21,125
V	2	-1372	-13,233	15,081
Cr	3	-1185	-10,000	11,397
Mn	4	-1037	-7,760	8,844
Fe	5	-910	-6,044	6,888
Co	6	-824	-5,073	5,782
Ni	7	-744	-4,201	4,787
Cu	8	-673	-3,492	3,979
Zn	9	-611	-2,917	3,325

X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-1275	-18,782	21,405
Cr	2	-1061	-11,832	13,485
Mn	3	-1007	-11,230	12,799
Fe	4	-812	-7,170	8,171
Co	5	-748	-5,905	6,730
Ni	6	-678	-4,749	5,412
Cu	7	-612	-3,762	4,288
Zn	8	-555	-2,887	3,290
Ga	9	-470	-1,875	2,137

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	1006	-62,636	74,865
Ti	2	786	-38,713	46,271
V	3	647	-26,551	31,734
Cr	4	544	-19,071	22,794
Mn	5	461	-13,867	16,575
Fe	6	409	-11,183	13,366
Co	7	360	-8,868	10,599
Ni	8	319	-7,073	8,455
Cu	9	284	-5,684	6,794

X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	583	-19,797	23,662
V	2	490	-14,133	16,892
Cr	3	423	-10,680	12,766
Mn	4	370	-8,288	9,906
Fe	5	325	-6,455	7,716
Co	6	295	-5,418	6,476
Ni	7	266	-4,486	5,362
Cu	8	240	-3,729	4,457
Zn	9	218	-3,116	3,724

X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	456	-20,060	23,976
Cr	2	379	-12,637	15,104
Mn	3	360	-11,994	14,336
Fe	4	290	-7,658	9,153
Co	5	267	-6,307	7,538
Ni	6	242	-5,072	6,062
Cu	7	219	-4,018	4,803
Zn	8	198	-3,083	3,685
Ca	9	168	-2,003	2,394

12.3.3 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for Sc (C_{3i}) site of $Na_3Sc_2Li_3F_{12}$ for transition-metal ions with electronic configuration $3d^N$

(a) For monopole A_{nm}					(b) For total A_{nm}				
X^{2+}	N	B_{20}	B_{40}	B_{43}	X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-148	41,243	-48,020	Sc	1	-422	-44,842	54,249
Ti	2	-116	25,491	-29,679	Ti	2	-330	-27,715	33,529
V	3	-95	17,482	-20,355	V	3	-271	-19,008	22,995
Cr	4	-80	12,557	-14,620	Cr	4	-228	-13,653	16,517
Mn	5	-68	9,131	-10,631	Mn	5	-193	-9,928	12,010
Fe	6	-60	7,363	-8,573	Fe	6	-171	-8,006	9,685
Co	7	-53	5,839	-6,798	Co	7	-151	-6,349	7,680
Ni	8	-47	4,658	-5,423	Ni	8	-134	-5,064	6,126
Cu	9	-42	3,743	-4,358	Cu	9	-119	-4,069	4,923
X^{3+}	N	B_{20}	B_{40}	B_{43}	X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-86	13,035	-15,177	Ti	1	-245	-14,173	17,146
V	2	-72	9,306	-10,835	V	2	-206	-10,118	12,241
Cr	3	-62	7,033	-8,188	Cr	3	-177	-7,646	9,250
Mn	4	-54	5,457	-6,354	Mn	4	-155	-5,934	7,178
Fe	5	-48	4,251	-4,949	Fe	5	-136	-4,621	5,591
Co	6	-43	3,568	-4,154	Co	6	-124	-3,879	4,693
Ni	7	-39	2,954	-3,440	Ni	7	-111	-3,212	3,886
Cu	8	-35	2,456	-2,859	Cu	8	-101	-2,670	3,230
Zn	9	-32	2,052	-2,389	Zn	9	-91	-2,231	2,698
X^{4+}	N	B_{20}	B_{40}	B_{43}	X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-67	13,208	-15,379	V	1	-191	-14,361	17,374
Cr	2	-56	8,321	-9,688	Cr	2	-159	-9,047	10,945
Mn	3	-53	7,898	-9,195	Mn	3	-151	-8,587	10,388
Fe	4	-43	5,042	-5,871	Fe	4	-122	-5,482	6,632
Co	5	-39	4,153	-4,835	Co	5	-112	-4,515	5,462
Ni	6	-36	3,340	-3,889	Ni	6	-102	-3,631	4,393
Cu	7	-32	2,646	-3,081	Cu	7	-92	-2,877	3,480
Zn	8	-29	2,030	-2,364	Zn	8	-83	-2,207	2,670
Ga	9	-25	1,319	-1,536	Ga	9	-70	-1,434	1,735

12.3.4 Theoretical crystal-field parameters, B_{nm} (cm^{-1}), for In (C_{3i}) site of $Na_3In_2Li_3F_{12}$ for transition-metal ions with electronic configuration $3d^N$

(a) For monopole A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-169	-37,086	43,785
Ti	2	-132	-22,922	27,062
V	3	-109	-15,720	18,560
Cr	4	-92	-11,291	13,331
Mn	5	-78	-8,211	9,694
Fe	6	-69	-6,621	7,817
Co	7	-61	-5,250	6,199
Ni	8	-54	-4,188	4,945
Cu	9	-48	-3,366	3,973
X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-98	-11,722	13,839
V	2	-82	-8,368	9,879
Cr	3	-71	-6,324	7,466
Mn	4	-62	-4,907	5,794
Fe	5	-55	-3,822	4,512
Co	6	-50	-3,208	3,788
Ni	7	-45	-2,656	3,136
Cu	8	-40	-2,208	2,607
Zn	9	-37	-1,845	2,178
X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-77	-11,877	14,022
Cr	2	-64	-7,482	8,834
Mn	3	-61	-7,102	8,384
Fe	4	-49	-4,534	5,353
Co	5	-45	-3,734	4,409
Ni	6	-41	-3,003	3,546
Cu	7	-37	-2,379	2,809
Zn	8	-33	-1,826	2,155
Ga	9	-28	-1,186	1,400

(b) For total A_{nm}

X^{2+}	N	B_{20}	B_{40}	B_{43}
Sc	1	-562	-40,793	49,455
Ti	2	-518	-25,213	30,566
V	3	-426	-17,292	20,963
Cr	4	-358	-12,420	15,057
Mn	5	-304	-9,031	10,949
Fe	6	-269	-7,283	8,829
Co	7	-237	-5,775	7,002
Ni	8	-210	-4,607	5,585
Cu	9	-187	-3,702	4,488
X^{3+}	N	B_{20}	B_{40}	B_{43}
Ti	1	-384	-12,893	15,631
V	2	-323	-9,204	11,159
Cr	3	-279	-6,956	8,433
Mn	4	-244	-5,398	6,544
Fe	5	-214	-4,204	5,097
Co	6	-194	-3,529	4,278
Ni	7	-175	-2,922	3,542
Cu	8	-158	-2,429	2,944
Zn	9	-144	-2,029	2,460
X^{4+}	N	B_{20}	B_{40}	B_{43}
V	1	-300	-13,064	15,838
Cr	2	-250	-8,230	9,978
Mn	3	-237	-7,811	9,470
Fe	4	191	-4,987	6,046
Co	5	-176	-4,108	4,980
Ni	6	-159	-3,303	4,005
Cu	7	-144	-2,617	3,173
Zn	8	-131	-2,008	2,434
Ga	9	-111	-1,304	1,581

12.4 Experimental Parameters (cm^{-1}) for Cr^{3+} in $Na_3M_2Li_3F_{12}$

M	$F^{(2)}$	$F^{(4)}$	B_{20}	B_{40}	B_{43}	Ref
In	59,696	42,714	0	-22,218[a]	--	5
Ga	59,973	42,242	0	-22,988[a]	--	1

[a]Cubic approx. $B_{43} = \sqrt{10/7}|B_{40}|$

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13. Cs_2SnBr_6

13.1 Crystallographic Data on Cs_2SnBr_6

Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x^a	y	z	q	$\alpha(Å^3)$
Sn	4(a)	O_h	0	0	0	4	0.37^b
Cs	8(c)	T_d	1/4	1/4	1/4	1	2.492^c
Br	24(e)	C_{4v}	x	0	0	-1	3.263^c

[a]X-ray data: a = 10.81 Å, x = 0.245 (reference 7).
[b]Reference 5.
[c]Reference 6.

13.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$), for Sn (O_h) Site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{40}	3325.2	-2255.7	5087.6	6157.0
A_{44}	1987.2	-1348.0	3040.4	3679.5

13.3 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}	Ref
Os^{4+}	$5d^4$	88,308	34,676	3212	10,096	4

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14. $KMgF_3$

14.1 Crystallographic Data on $KMgF_3$

Cubic O_h^1 (Pm3m), 221, Z = 1

Ion	Site	Symmetry	x[a]	y	z	q	α ($Å^3$)[b]
K	1(a)	O_h	0	0	0	1	0.827
Mg	1(b)	O_h	1/2	1/2	1/2	2	0.0809
F	3(d)	D_{4h}	1/2	1/2	0	-1	0.731

[a]X-ray data: a = 3.973 Å (reference 33).
[b]Reference 25.

14.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$), for Mg (O_h) (1b) Site

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{40}	13,281	-5022	0	8260
A_{44}	7,937	-3001	0	4936

14.3 Experimental Parameters (cm^{-1})

Ion	$F^{(2)}$	$F^{(4)}$	ζ	α	B_{40}[a]	Ref.
V^{2+}	53,362	28,065	--	79	25,515	29
Co^{2+}	70,224	48,787	500	--	16,800	6
Ni^{2+}	74,480	50,274	620	--	14,658	4
Mn^{2+}	64,099	38,983	0	0	18,659	29
Ni^{2+}	76,405	53,298	--	--	15,225	13
Ni^{2+}	74,270	49,322	--	--	15,909	(b)

[a]$B_{44} = \sqrt{5/14}\, B_{40}$
[b]Best fit to the data (reference 31) with $F^{(2)}$, $F^{(4)}$, and B_{40} varied.

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15. $BeAl_2O_4$ (Chrysoberyl, $Cr:BeAl_2O_4$ = Alexandrite)

15.1 Crystallographic Data on $BeAl_2O_4$

Orthorhombic D_{2h}^{16} (Pnma), 62, Z = 4

Ion	Site	Symmetry	x	y	z	q	α (Å^3)[a]
Al_1	4(a)	C_i	0	0	0	3	0.0530
Al_2	4(c)	C_s	x	1/4	z	3	0.0530
Be	4(c)	C_s	x	1/4	z	2	0.0125
O_1	4(c)	C_s	x	1/4	z	-2	1.349
O_2	4(c)	C_s	x	1/4	z	-2	1.349
O_3	8(d)	C_1	x	y	z	-2	1.349

[a]Reference 15.

15.2 X-Ray Data

Cell size			Al_2		Be	
a	b	c	x	z	x	z
9.4041	5.4756	4.4267	0.27319	-0.00595	0.09294	0.43347
9.407	5.4781	4.4285	0.27283	-0.00506	0.09276	0.43402

O_1		O_2		O_3			Ref.
x	z	x	z	x	y	z	
0.09051	0.79016	0.43343	0.24097	0.16318	0.01718	0.25850	28
0.09031	0.78779	0.43302	0.24137	0.16330	0.01529	0.25687	3

15.3 Crystal-Field Components

A_{nm} ($cm^{-1}/Å^n$) for Al_2 (C_s) site (rotated so that z-axis is perpendicular to mirror plane)

Calculated using data from reference 28

A_{nm}	Monopole	Total
ReA_{11}	-1,474	-2533
ImA_{11}	-5,753	-1586
A_{20}	4,776	-658.4
A_{22}	5,573	6129
ReA_{31}	6,459	3852
ImA_{31}	-7,028	3936
ReA_{33}	-4,503	-346.7
ImA_{33}	-1,662	46.55
A_{40}	-4,588	-1744
ReA_{42}	-18,247	-2571
ImA_{42}	-12,176	8657
ReA_{44}	4,922	-3188
ImA_{44}	11,144	-4138
ReA_{51}	180.6	322.5
ImA_{51}	-2,189	1879
ReA_{53}	-1,037	1287
ImA_{53}	-1,271	-687.8
ReA_{55}	-1,674	812.1
ImA_{55}	360.7	1159

Calculated using data from reference 3

A_{nm}	Monopole	Total
ReA_{11}	-1,247	-2303
ImA_{11}	6,656	-1410
A_{20}	4,828	-471.4
A_{22}	5,584	5661
ReA_{31}	6,754	3340
ImA_{31}	-6,192	3415
ReA_{33}	-4,408	-79.97
ImA_{33}	-2,256	-50.58
A_{40}	-4,872	-1994
ReA_{42}	-17,366	-2231
ImA_{42}	-13,550	8786
ReA_{44}	3,246	-3544
ImA_{44}	11,736	-3798
ReA_{51}	153.9	378.6
ImA_{51}	-1,991	1914
ReA_{53}	-969.5	1295
ImA_{53}	-1,395	-849.1
ReA_{55}	-1,566	984.6
ImA_{55}	42.10	994.5

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16. $ZnAl_2O_4$

16.1 Crystallographic Data on $ZnAl_2O_4$

Cubic O_h^7 (Fd3m), 227, Z = 8

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)^b
Zn	8(a)	T_d	0	0	0	2	0.676
Al	16(d)	D_{3d}	5/8	5/8	5/8	3	0.0530
O	32(e)	C_{3v}	x	x	x	-2	1.349

[a]X-ray data: a = 8.0883 Å, x = 0.390 (reference 13).
[b]Reference 10.

16.2 Crystal Fields for Zn (T_d) Site

16.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Zn (T_d) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{32}	-i27,467	i7189	i6951	-i1,327
A_{40}	-12,005	4187	4544	-3,274
A_{44}	-7,174	2502	2716	-1,956

$i = \sqrt{-1}$

16.2.2 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Al (D_{3d}) site (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	5,004	22,132	-2576	24,559
A_{40}	-21,556	-3,990	9380	-16,162
A_{43}	24,259	1,899	-9322	16,830

16.3 Experimental Values (cm^{-1}) of $F^{(2)}$, $F^{(4)}$, α, ζ, and B_{nm} for nd^N Ions

Ion	d^N	$F^{(2)}$	$F^{(4)}$	α	ζ	B_{20}	B_{40}	B_{44}	B_{43}	Ref.
Co^{2+}	$3d^7$	59,367	42,210	86	420	--	-8,640	5145.46	--	9
Cr^{3+}	$3d^3$	56,700	40,320	--	250	4608	-30,625	--	28,415	3,7,12

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17. $LiMgZrO_4$

17.1 Crystallographic Data on $LiMgZrO_4$

Tetragonal ($I4_1/amd$), 141 (second setting), Z = 2

Ion	Site	Symmetry	x^a	y	z	q	α (Å^3)
O	8(e)	C_{2v}	0	1/4	0.108	-2	1.349
Zr,Mg	4(a)	D_{2d}	0	3/4	1/8	4,2	0.280
Li	4(b)	D_{2d}	0	1/4	3/8	1	0.0321

[a]X-ray data: a = 4.209 Å, c = 9.145 Å (reference 1).

17.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$) for 4a (D_{2d}) Site

Assuming that average charge on site 4(a) is +3

A_{nm}

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	-4,837	99.2	13,303	8,564
A_{32}	618.0	-854.3	4,448	4,212
A_{40}	19,053	-5338	2,835	16,550
A_{44}	11,142	-3404	-430.3	7,308
A_{52}	-1,763	599.6	-1,229	-2,393

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18. $La_3Lu_2Ga_3O_{12}$

18.1 Crystallographic Data on $La_3Lu_2Ga_3O_{12}$

Cubic O_h^{10} (Ia3d), 230, Z = 8

Ion	Site	Symmetry	x[a]	y	z	q	α (Å^3)[b]
La	24(c)	D_2	0	1/4	1/8	3	1.41
Lu	16(a)	C_{3i}	0	0	0	3	0.77
Ga	24(d)	S_4	0	1/4	3/8	3	0.458
O	96(h)	C_1	-0.02976	0.05819	0.15699	-2	1.349

[a]X-ray data: a = 12.93 (reference 1).
[b]Values for α are from reference 6, and for values not given there, the α values are from reference 2.

18.2 Crystal-Field Components, A_{nm} (cm^{-1}/Å^n)

18.2.1 For Ga ion in 24(d) (S_4) site

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	10,298	-2189	8197	16,306
ReA_{32}	-14,919	4063	-7814	-18,670
ImA_{32}	32,502	-8342	6011	30,171
A_{40}	-18,159	7076	-5524	-16,607
ReA_{44}	-4,696	1758	4006	-2,538
ImA_{44}	-5,156	2214	-2319	-5,260
ReA_{52}	-1,758	1130	-1683	-2,311
ImA_{52}	3,807	-2351	2290	3,475

18.2.2 For Lu ion in 16(a) (C_{3i}) site (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	8,619	-839	-9970	-2190
A_{40}	-10,698	3041	8056	-6852
ReA_{43}	600	-316	2583	2867
ImA_{43}	-11,521	3056	-13	-8478

$La_3Lu_2Ga_3O_{12}$

18.2.3 For La ion in 24(c) (D_2) site[a]

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	-1196	-369	11,910	10,345
A_{22}	1305	-155	-107	43
A_{32}	-i1029	-i34	i1,453	i390
A_{40}	-663	-70	-20	-753
A_{42}	5073	-990	-323	3,760
A_{44}	-2522	530	971	-1,021
A_{52}	i1783	-i477	i106	i1,414
A_{54}	i967	-i253	-i87	i627
A_{60}	-1203	336	4	-863
A_{62}	549	-213	200	536
A_{64}	567	-193	-235	139
A_{66}	-474	166	202	106
A_{72}	-i73	i32	i124	i83
A_{74}	i106	-i60	i68	i114
A_{76}	i159	-i54	-i43	i62

[a] $i = \sqrt{-1}$

18.3 Experimental Parameters (cm^{-1})

Ion	Symmetry	$F^{(2)}$	$F^{(4)}$	B_{40}	T	Ref.
Cr^{3+}	C_{3i}	49,830	35,097	-20,720	4 K	7

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19. ZnO

19.1 Crystallographic Data on ZnO

Hexagonal C_{6v}^{4} ($P6_3mc$), 186, Z = 2

Ion	Site	Symmetry	x	y	z	q	α (A^3)[a]
Zn	2(b)	C_{3v}	1/3	2/3	0	2	0.676
O	2(b)	C_{3v}	1/3	2/3	z	-2	1.349

[a]Reference 24.

19.2 X-Ray Data

a	c	z	Ref.
3.24950	5.2069	0.345	30
3.24270	5.1948	0.3826	23
3.24968	5.20662	0.3825	1

19.3 Crystal-Field Components, A_{nm} (cm^{-1}/A^n), for Zn (C_{3v}) Site

Calculated using data from reference 30

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{10}	31,224	0	7,662	38,886
A_{20}	17,809	-2,962	22,891	37,738
A_{30}	36,957	-9,440	8,892	36,409
A_{33}	15,279	-3,287	-4,742	7,249
A_{40}	10,043	-5,353	4,269	8,959
A_{43}	-8,681	2,903	1,141	-4,637
A_{50}	4,136	-3,662	6,358	6,831
A_{53}	39.7	-578.3	1,254	1,415

Calculated using data from reference 23

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{10}	28,160	0	-311.5	27,849
A_{20}	-1,685	254.0	14,628	13,197
A_{30}	29,882	-6,758	6,088	29,211
A_{33}	20,084	-4,709	-3,930	11,446
A_{40}	8,622	-3,384	-449.8	-5,885
A_{43}	-9,102	3,384	-167.6	-5,885
A_{50}	-551.3	269.1	2,694	2,411
A_{53}	-886.2	250.6	1,696	1,060

Calculated using data from reference 1

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{10}	28,033	0	-293.4	27,740
A_{20}	-1,631	244.7	14,444	13,058
A_{30}	29,635	-6658	5,992	28,968
A_{33}	19,895	-4633	-3,870	11,392
A_{40}	8,522	-3148	-435.8	4,938
A_{43}	-9,003	3325	-161.1	-5,840
A_{50}	-536.4	258.1	2,646	2,368
A_{53}	-868.7	242.5	1,661	1,035

19.4 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	α	β	ζ	B_{20}	B_{40}	B_{43}	Ref.
Ni^{2+}	$3d^8$	63,630	46,620	--	--	500	95.69	7072	6529	2
Ni^{2+}	$3d^8$	63,602	46,570	--	--	500	--	5880	7028	29[a]
Ni^{2+}	$3d^8$	63,218	43,674	--	--	630	--	5670	6777	20[a]
Co^{2+}	$3d^7$	62,388	43,943	--	--	630	--	5460	6526	29[a]
Co^{2+}	$3d^7$	61,250	44,100	--	--	450	-590	4077	7331	16
Co^{2+}	$3d^7$	56,350	39,690	--	--	540	--	5460	6526	11[a]
Cu^{3+}	$3d^9$	--	--	--	--	--	--	7000	8367	29[a]

[a]Cubic, $B_{20} = 0$, $B_{43} = \sqrt{10/7}\,|B_{40}|$

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20. ZnS

20.1 Crystallographic Data on ZnS

20.1.1 Cubic T_d^2 ($F\bar{4}3m$), 216, Z = 4

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)[b]
Zn	4a	T_d	0	0	0	2	0.676
S	4c	T_d	1/4	1/4	1/4	-2	4.893

[a]X-ray data: a = 5.4093 Å (reference 32, p 110).
[b]Reference 20.

20.1.2 Hexagonal C_{6v}^4 ($P6_3mc$), 186, Z = 2

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)
Zn	2(b)	C_{3v}	1/3	2/3	0	2	0.676
S	2(b)	C_{3v}	1/3	2/3	z	-2	4.893

[a]X-ray data: a = 3.811 Å, c = 6.234 Å (reference 32, p 112).

20.2 Crystal Fields

20.2.1 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Zn (T_d) site of cubic ZnS

A_{nm}	Monopole	Self-induced	Total
A_{32}	15,219	-7349	7869
A_{40}	-4,610	4035	-574.8
A_{44}	2,755	-2411	343.5

20.2.2 Crystal-field components, A_{nm} ($cm^{-1}/Å^n$), for Zn (C_{3v}) site of hexagonal ZnS

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{10}	20,496	0	9,537	30,033
A_{20}	10,188	-3,463	26,174	32,899
A_{30}	18,608	-10,166	7,716	16,158
A_{33}	7,926	-3,754	-4,809	-636.8
A_{40}	3,800	-4,417	3,128	2,511
A_{43}	-3,877	2,887	952.3	-37.21
A_{50}	1,334	-2,505	4,341	3,171
A_{53}	339.5	-518.3	874.1	695.3

20.3 Experimental Values (cm^{-1}) of $F^{(2)}$, $F^{(4)}$, ζ, and B_{40} for $3d^N$ Ions

Ion	$3d^N$	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}[a]	Ref
V^{2+}	$3d^3$	--	--	--	-10,326	8
Cr^{2+}	$3d^4$	81,148	31,529	--	-10,924	6
Mn^{2+}	$3d^5$	44,280	43,981	--	-10,351	7
Mn^{2+}	$3d^5$	56,454	32,925	--	-11,603	22
Fe^{2+}	$3d^6$	51,433	36,195	--	-7,486	24,10
Co^{2+}	$3d^7$	49,516	35,438	583	-7,897	31
Co^{2+}	$3d^7$	53,851	40,619	--	-7,509	15
Ni^{2+}	$3d^8$	46,449	32,211	477	-9,321	31
Ni^{2+}	$3d^8$	50,119	29,445	--	-10,701	19

[a] $B_{44} = \sqrt{5/14}\,|B_{40}|$, $Dq = 21|B_{40}|$

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21. K_2PtCl_6

21.1 Crystallographic Data on K_2PtCl_6

Cubic O_h^5 (Fm3m) 225, Z = 4

Ion	Site	Symmetry	x^a	y	z	q	α (A^3)
Pt	4(a)	O_h	0	0	0	4	0.67[b]
K	8(c)	T_d	1/4	1/4	1/4	1	0.827[c]
Cl	24(e)	C_{4v}	x	0	0	-1	2.694[c]

[a]X-ray data: a = 9.755 A, x = 0.240 (reference 12).
[b]Reference 5.
[c]Reference 10.

21.2 Crystal-Field Components, A_{nm} (cm^{-1}/A^n), for Pt (O_h) Site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{40}	6115.0	-5016.9	10,480	11,578
A_{44}	3654.4	-2998.2	6,262.7	6,919.0

21.3 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}	Ref.
Ru^{4+}	$4d^4$	48,888	17,174	1044	39,732	9
Re^{4+}	$5d^3$	28,749	22,907	2392	63,729	4
Os^{4+}	$5d^4$	45,381	16,330	2416	47,229	3
Re^{4+}	$5d^3$	28,843	22,582	2360	63,477	6
Re^{4+}	$5d^3$	29,963	22,907	2392	63,729	14

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22. $Y_3Ga_5O_{12}$ (YGG)

22.1 Crystallographic Data on $Y_3Ga_5O_{12}$

Cubic O (Ia3d), 230, Z = 8

Ion	Site	Symmetry	x[a]	y	z	q	α ($Å^3$)[b]
Y	24(c)	D_2	0	1/4	1/8	3	0.870
Ga_1	16(a)	C_{3i}	0	0	0	3	0.458
Ga_2	24(d)	S_4	0	1/4	3/8	3	0.458
O	96(h)	C_1	-0.0272	0.05580	0.1501	-2	1.349

[a]X-ray data: a = 12.28 (reference 5).
[b]Reference 10.

22.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$)

22.2.1 For Ga ion in 24(d) (S_4) site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	7,529.074	-2139.311	9280.060	14,669.823
ReA_{32}	-19,875.040	5487.624	-9440.532	-23,827.948
ImA_{32}	32,745.166	-8848.915	5910.520	29,806.771
A_{40}	-19,871.204	8061.824	-6493.768	-18,303.148
ReA_{44}	-3,959.054	1499.466	1011.514	-1,448.074
ImA_{44}	-6,410.529	2934.927	-2624.400	-6,100.002
ReA_{52}	-2,135.999	1448.737	-2204.848	-2,892.110
ImA_{52}	3,718.967	-2388.618	2509.017	3,839.366
$\|A_{44}\|$	7,534.52	--	--	6,269.525

22.2.2 For Ga_1 ion in 16(a) (C_{3i}) site (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	15,183.2	-1576.3	-14,849	-1,242.3
A_{40}	-17,783.6	6625.2	1,754.4	-9,403.4
ReA_{43}	1,294.6	-745.1	4,955.7	5,505.3
ImA_{43}	-18,677.5	6650.8	530.7	-11,496
$\|A_{44}\|$	18,722	--	--	12,746

22.3 Experimental Parameters (cm^{-1})

$F^{(2)}$	$F^{(4)}$	B_{20}	B_{40}	B_{43}	Ref.
53,994	40,735	--	-22,820[a]	--	11[b]
54,638	40,456	--	-21,140[a]	--	11[c]

[a]Cubic approximation $B_{43} = \sqrt{10/7}\ |B_{40}|$.
[b]Fit to E_0 data of reference 11.
[c]Fit to E_a data of reference 11.

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23. $La_{2-x}Sr_xCuO_4$

23.1 Crystallographic Data on $La_{1.85}Sr_{0.15}CuO_4$

23.1.1 Tetragonal, D_{4h}^{17} (I4/mmm), 139, Z = 2; T = 300 K

Ion	Site	Symmetry	x	y	z	q^a	q^b
La/Sr	4(e)	C_{4v}	0	0	z	2.775	2.925
Cu	2(a)	D_{4h}	0	0	0	2.45	2.15
O_1	4(e)	C_{4v}	0	0	z	-2	-2
O_2	4(c)	D_{2h}	0	1/2	0	-2	-2

[a]The effective charges on the Cu ions are chosen as 55% Cu^{2+} + 45% Cu^{3+}, and the total charge in the unit cell vanishes.
[b]The charge on La is taken as 3 and the charge on Sr is taken as 2, so that the average charge on the La/Sr site is [3(1.85) + 2(0.15)]/2. The charge on the Cu ion is then chosen so that the total charge in a unit cell is zero.

23.1.2 Orthorhombic D_{2h}^{18} (Cmca), 64, Z = 4; T = 10 K and 60 K

Ion	Site	Symmetry	x	y	z	q^a	q^b
La/Sr	8(f)	C_s	0	y	z	2.775	2.925
Cu	4(a)	C_{2h}	0	0	0	2.450	2.15
O_1	8(f)	C_s	0	y	z	-2	-2
O_2	8(e)	C_2	1/4	y	1/4	-2	-2

[a,b]See notes to 23.1.1

23.2 X-Ray Data

23.2.1 Tetragonal, T = 300 K

a	c	Z_{La}	Z_{O_1}	Ref
3.7793	13.226	0.36046	0.1824	1
3.7749	13.2231	0.3606	0.1826	3

23.2.2 Orthorhombic, T = 10 K and 60 K

Temp	a	b	c	y_{La}	z_{La}	y_{O_1}	z_{O_2}	y_{O_2}
10 K	5.3240	13.1832	5.3547	-0.36077	-0.00496	-0.18260	0.0255	-0.00573
60 K	5.3252	13.1844	5.3546	-0.36072	-0.00495	-0.18257	0.0256	-0.00560

Reference 1 (transformed to the standard in the International Tables).

23.3 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$)

23.3.1 For La (C_{4v}) site in tetragonal $La_{1.85}Sr_{0.15}CuO_4$

A_{nm}	300 K (ref 1)	300 K (ref 2)
A_{10}	-6369	4915
A_{20}	8888	9248
A_{30}	-4634	-5675
A_{40}	1954	1451
A_{44}	-1773	-1818
A_{50}	-3188	-3127
A_{54}	1691	1590
A_{60}	364.2	358.4
A_{64}	745.9	720.3
A_{70}	136.4	-123.5
A_{74}	76.61	77.69

23.3.2 For La (C_s) site of orthorhombic $La_{1.85}Sr_{0.15}CuO_4$ rotated so that z-axis of A_{nm} is parallel to b-axis and A_{22} is real and positive

A_{nm}	60 K	10 K
ReA_{11}	3904	3919
ImA_{11}	6897	6952
A_{20}	-4544	-4534
A_{22}	5272	5284
ReA_{31}	-2027	-2023
ImA_{31}	-30.36	-26.08
ReA_{33}	2759	2760
ImA_{33}	-187.2	-149.7
A_{40}	2573	2567
ReA_{42}	496.0	499.0
ImA_{42}	-184.5	-189.9
ReA_{44}	1444	1439
ImA_{44}	-260.8	-245.5

For La (C_s) site (cont'd)

A_{nm}	60 K	10 K
ReA_{51}	2070	1992
ImA_{51}	366.8	359.0
ReA_{53}	48.29	-104.4
ImA_{53}	466.5	407.40
ReA_{55}	1657	1711
ImA_{55}	1010	1084
A_{60}	404.8	405.6
ReA_{62}	-46.89	-47.26
ImA_{62}	81.61	82.61
ReA_{64}	-688.5	-685.5
ImA_{64}	-305.5	-314.3
ReA_{66}	-22.47	-22.21
ImA_{66}	-32.74	-32.38
ReA_{71}	-83.33	-83.31
ImA_{71}	-2.75	-2.87
ReA_{73}	38.85	39.08
ImA_{73}	-27.77	-27.61
ReA_{75}	9.35	9.67
ImA_{75}	20.60	20.67
ReA_{77}	85.19	84.98
ImA_{77}	13.54	15.27

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24. Al_2O_3 (Corundum)

24.1 Crystallographic Data on Al_2O_3

Hexagonal D_{3d}^6 (R3c) (second setting), 167, Z = 6

Ion	Site	Symmetry	x	y	z	q	α ($Å^3$)
Al	12(c)	C_3	0	0	z	3	0.053
O	18(e)	C_2	x	0	1/4	-2	1.349

24.2 X-Ray Data

a	c	z_{Al}	x_O	Ref	Set
4.7628	13.0032	0.352	0.306	37	1
4.7586	12.9897	0.3518	0.6918	51	2
4.75855	12.9906	0.35200	0.6936	51	3
4.75999	12.99481	0.35219	0.69367	51	4
4.7640	13.0091	0.35221	0.30636	12	5

24.3 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$), for Al (C_3) Site

Set 1

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{10}	6,472	--	-6424	48.41
A_{20}	-4,896	778.2	1933	-2,185
A_{30}	-9,718	4215	620.4	-4,883
Re A_{33}	-639.7	-1220	1126	-733.6
Im A_{33}	-10,955	3434	1253	-6,268
A_{40}	-18,418	6479	-66.36	-12,005
Re A_{43}	4,371	-1322	629.3	3,678
Im A_{43}	-23,006	9736	417.6	-12,853
A_{50}	8,476	-4130	458.8	4,804
Re A_{53}	1,581	-486.9	107.8	1,201
Im A_{53}	1,766	-592.6	798.9	1,973

Al_2O_3

Set 2

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{10}	8,456	--	-6841	615
A_{20}	-5,475	852.5	2003	-2,619
A_{30}	-9,692	4327	695.7	-4,669
Re A_{33}	-1,050	-1147	1241	-955.1
In A_{33}	11,217	-3561	-1337	6,319
A_{40}	-18,612	6555	-65.65	-12,123
Re A_{43}	4,167	-1252	706.9	3,622
Im A_{43}	23,259	-9890	-440.6	12,928
A_{50}	8,352	-4057	487.9	4,783
Re A_{53}	1,564	-470.9	128.8	1,222
Im A_{53}	-1,543	413.5	-861.5	-1,991

Set 3

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{10}	6,840	--	-6447	393.1
A_{20}	-5,026	799.8	1933	-2,293
A_{30}	-9,783	4267	629.7	-4,886
Re A_{33}	-704.1	-1214	1140	-778.5
Im A_{33}	11,064	-3485	-1261	6,318
A_{40}	-18,498	6524	-64.96	-12,039
Re A_{43}	4,355	-1319	639.6	3,676
Im A_{43}	23,136	-9822	-420.9	12,893
A_{50}	8,497	-4150	460.7	4,808
Re A_{53}	1,583	-487.1	110.6	1,206
Im A_{53}	-1,733	561.8	-805.5	-1,976

Set 4

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{10}	6,774	--	-6442	331.9
A_{20}	-5,000	795.2	1933	-2,272
A_{30}	-9,766	4253	627.7	-4,885
Re A_{33}	-692.5	-1214	1137	-769.6
Im A_{33}	11,039	-3473	-1259	6,307
A_{40}	-18,471	6509	-65.14	-12,027
Re A_{43}	4,355	-1318	637.4	3,675
Im A_{43}	23,096	-9795	-420.1	12,880
A_{50}	8,486	-4141	460.0	4,805
Re A_{53}	1,581	-486.5	110.1	1,205
Im A_{53}	-1,737	566.4	-803.7	-1,974

Set 5

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{10}	6,778	--	-5821	957.6
A_{20}	-5,003	813.0	1753	-2,437
A_{30}	-10,007	4292	564.1	-5,151
Re A_{33}	-634.0	-1213	1033	-813.9
Im A_{33}	-11,173	3512	1140	-6,521
A_{40}	-18,251	6420	-51.53	-11,882
Re A_{43}	4,361	-1314	577.4	3,625
Im A_{43}	-22,971	9724	387.6	-12,860
A_{50}	8,469	-4134	408.8	4,744
Re A_{53}	1,563	-481.0	98.52	1,180
Im A_{53}	1,709	-539.5	720.8	1,891

24.4 Experimental Parameters (cm^{-1}) for Transition-Metal Ions

Ion	nd^N	Site	$F^{(2)}$	$F^{(4)}$	α	ζ	B_{20}	B_{40}	B_{43}	Ref
V^{3+}	$3d^2$	Al	47,390	31,500	--	155	234	-23,564	30,803	25
Cr^{3+}	$3d^3$	Al	53,690	39,312	--	170	-1123	-22,350	31,538	26

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25. $MgAl_2O_4$

25.1 Crystallographic Data on $MgAl_2O_4$

Cubic O_h^7 (Fd3m), 227, Z = 8

Ion	Site	Symmetry	x[a]	y	z	q	α (A^3)[b]
Mg	8(a)	T_d	0	0	0	2	0.0809
Al	16(d)	D_{3d}	5/8	5/8	5/8	3	0.053
O	32(e)	C_{3v}	x	x	x	-2	1.349

[a]X-ray data: a = 8.080 A, x = 0.389 (reference 10).
[b]Reference 6.

25.2 Crystal-Field Components, A_{nm} (cm^{-1}/A^n)

25.2.1 For Al (D_{3d}) site (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	-2,283	-2008	23,088	18,797
A_{40}	-20,238	8618	-4,838	-16,458
A_{43}	23,688	-8781	2,390	17,297

25.2.2 For Mg (T_d) site

A_{nm}	Point-charge	Self-induced	Dipole	Total
A_{32}	30,202	-8210	-9151	12,840
A_{40}	-13,597	5447	5350	-2,800
A_{44}	8,126	-3255	-3197	1,673

25.3 Experimental Parameters (cm^{-1}) for Transition-Metal Ions

Ion	nd^N	Site	$F^{(2)}$	$F^{(4)}$	α	ζ	B_{20}	B_{40}	B_{4m}[a]	Ref.
Cr^{3+}	$3d^3$	Al	56,700	40,320	--	250	4608	-30,625	28,415	9
Cr^{3+}	$3d^3$	Al	56,700	40,320	--	--	0	-25,550	30,538	9
Fe^{2+}	$3d^6$	Mg	--	--	--	-392	0	-9,387	--	7
Co^{2+}	$3d^7$	Mg	--	--	--	--	0	-8,400	--	1

[a]For Al site $B_{4m} = B_{43}$, and for Mg site $B_{4m} = B_{44}$ ($B_{44} = \sqrt{5/14}\,|B_{40}|$).

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26. $A_3^{+2}B_2^{+3}Ge_3O_{12}$ (Germanium Garnet)

26.1 Crystallographic Data on $A_3B_2Ge_3O_{12}$

Cubic O_h^{10} (Ia3d), 230, Z = 8

Ion	Site	Symmetry	x	y	z	q	α ($Å^3$)[a]
A^{+2}	24(c)	D_2	0	1/4	1/8	2	α_A
B^{+3}	16(a)	C_{3i}	0	0	0	3	α_B
Ge	24(d)	S_4	0	1/4	3/8	4	0.12
O	96(h)	C_1	x	y	z	-2	1.349

[a]Values for α are from reference 19, and for values not given there the α are from reference 3.

26.2 X-Ray Data on $A_3B_2Ge_3O_{12}$

A^{+2}	B^{+3}	a	x	y	z	Ref.	α_A[a]	α_B[a]
Ca	Al	12.118	-0.03345	0.0488	0.14753	22	0.564	0.0530
Ca	Ga	12.251	--	--	--	24	0.564	0.19
Ca	Cr	12.262	--	--	--	24	0.564	0.29
Ca	V	12.324	--	--	--	24	0.564	0.31
Ca	Fe	12.325	--	--	--	24	0.564	0.24
Ca	Sc	12.519	-0.0352	0.0524	0.1552	22	0.564	0.540
Ca	Lu	12.590	-0.03538	0.05607	0.15989	22	0.564	0.77
Ca	In	12.735	-0.0363	0.0543	0.15724	22	0.564	0.54
Sr	Sc	12.785	-0.03861	0.04909	0.15339	22	1.039	0.540
Cd	Sc	12.458	-0.03437	0.05300	0.15564	13	0.840	0.540
Cd	Al	12.08	--	--	--	24	0.840	0.0530
Cd	Cr	12.20	--	--	--	24	0.840	0.29
Cd	Fe	12.26	--	--	--	24	0.840	0.24
Cd	Ga	12.19	--	--	--	24	0.840	0.19
Mn	Al	11.902	--	--	--	24	0.460	0.0530
Mn	Cr	12.027	--	--	--	24	0.460	0.29
Mn	Fe	12.087	--	--	--	24	0.460	0.24
Mn	Ga	12.00	--	--	--	24	0.460	0.19

[a]Values for α are from reference 19, and for values not given there the α are from reference 3.

26.3 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$)

Rotated so that z-axis is parallel to (111) crystallographic axis

26.3.1 For Al ion in 16(a) (C_{3i}) site in $Ca_3Al_2Ge_3O_{12}$

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	11,161	-451.6	-35,565	-24,855
A_{40}	-20,669	8255	9,602	-2,812
ReA_{43}	2,625	-1473	7,554	8,706
ImA_{43}	-22,662	9272	5,206	-8,184
$\|A_{43}\|$	22,814	--	--	11,949

26.3.2 For Sc ion in 16(a) (C_{3i}) site in $Ca_3Sc_2Ge_3O_{12}$

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	9,208	-299.1	-28,304	-19,395
A_{40}	-13,449	4192	5,733	-3,523
ReA_{43}	1,227	-651.0	4,588	5,164
ImA_{43}	-14,541	4678	2,550	-7,313
$\|A_{43}\|$	14,593	--	--	8,953

26.3.3 For Lu ion in 16(a) (C_{3i}) site in $Ca_3Lu_2Ge_3O_{12}$

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	10,201	-354.1	-26,892	-17,044
A_{40}	-11,205	3133	4,153	-3,920
ReA_{43}	525.3	-376.6	3,896	4,044
ImA_{43}	-11,743	3417	1,241	-7,085
$\|A_{43}\|$	11,754	--	--	8,158

$A_3^{+2}B_2^{+3}Ge_3O_{12}$

26.3.4 For In ion in 16(a) (C_{3i}) site in $Ca_3In_2Ge_3O_{12}$

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	8,212	-237.9	-25,117	-17,143
A_{40}	-11,352	3214	4,616	-3,523
ReA_{43}	612.7	-398.0	3,909	4,123
ImA_{43}	-12,272	3594	1,839	-6,838
$\|A_{43}\|$	12,287	--	--	7,985

26.3.5 For Sc ion in 16(a) (C_{3i}) site in $Sr_3Sc_2Ge_3O_{12}$

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	2,456	79.17	-22,887	-20,343
A_{40}	-12,168	3,703	6,298	-2,167
ReA_{43}	1,424	-667.5	4,090	4,847
ImA_{43}	-14,278	4,414	3,785	-6,079
$\|A_{43}\|$	14,349	--	--	7,775

26.3.6 For Sc ion in 16(a) (C_{3i}) site in $Cd_3Sc_2Ge_3O_{12}$

A_{nm}	Point charge	Self-induced	Dipole	Total
A_{20}	10,782	-444.2	-29,570	-19,232
A_{40}	-13,735	4323	5,561	-3,851
ReA_{43}	1,236	-664.4	4,670	5,241
ImA_{43}	-14,599	4729	2,266	-7,605
$\|A_{43}\|$	14,652	--	--	9,236

26.4 Experimental Values (cm^{-1}) of B_{40}, $F^{(2)}$, and $F^{(4)}$ for nd^N Ions in $Ca_3Ga_2Ge_3O_{12}$

Ion	Site	nd^N	B_{40}	$F^{(2)}$	$F^{(4)}$	Ref.
Cr^{+3}	C_{3i}	$3d^3$	-21,200	66,121	31,102	14

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27. $ZnGa_2O_4$

27.1 Crystallographic Data on $ZnGa_2O_4$

Cubic O_h^7 (Fd3m), 227, Z = 8

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)^b
Zn	8(a)	T_d	0	0	0	2	0.676
Ga	16(d)	D_{3d}	5/8	5/8	5/8	3	0.458
O	32(e)	C_{3v}	x	x	x	-2	1.349

[a]X-ray data: a = 8.330 Å, x = 0.38675 (reference 5).
[b]Reference 10.

27.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$)

27.2.1 For Zn (T_d) site

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{32}	26,942	-7790	-6727	-12,425
A_{40}	-11,793	4419	4333	-3,040
A_{44}	7,047	-2641	-2590	1,817

27.2.2 For Ga (D_{3d}) site (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Dipole	Self-induced	Total
A_{20}	-2,616	19,928	-1736	15,576
A_{40}	-17,273	-3,972	6713	-14,531
A_{43}	20,288	1,969	-6815	15,442

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28. Cs_2GeF_6

28.1 Crystallographic Data on Cs_2GeF_6

Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x[a]	y	z	q	α ($Å^3$)
Ge	4(a)	O_h	0	0	0	4	0.120[b]
Cs	8(c)	T_d	1/4	1/4	1/4	1	2.492[c]
F	24(e)	C_{4v}	x	0	0	-1	0.731[c]

[a]X-ray data: a = 9.021 Å, x = 0.20 (reference 16).
[b]Reference 3.
[c]Reference 14.

28.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$)

28.2.1 For Ge (O_h) site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{40}	21,689	-10,895	25,645	36,439
A_{44}	12,962	-6,511.5	15,326	21,776

28.2.2 For Cs (T_d) site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{32}	1162.7	139.27	-2378.4	-1076.4
A_{40}	-181.65	43.06	-174.48	-313.07
A_{44}	108.56	-25.74	104.27	187.10

28.3 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}	Ref
Mn^{4+}	$3d^3$	52,794	50,929	380	45,885	1
Mn^{4+}	$3d^3$	58,489	48,460	363	45,780	17
Re^{4+}	$5d^3$	40,299	22,617	2953	73,143	8
Pt^{4+}	$5d^6$	35,133	28,400	3579	66,150	13
Os^{4+}	$5d^4$	51,408	37,409	2800	51,450	15
Ir^{4+}	$5d^5$	53,389	39,564	3500	51,450	15
Re^{4+}	$5d^3$	40,019	22,554	3094	69,384	9

Cs_2GeF_6

28.4 Index of Refraction

$n = 1.3920 + 2.26\nu^2 \times 10^{-11}$ (ν in cm^{-1}) (reference 7)

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29. $R_2Ti_2O_7$ (R ≠ Y)

29.1 Crystallographic Data on $R_2Ti_2O_7$

Cubic O_h^7 (Fd3m), 227 (second setting), Z = 8

Ion	Site	Symmetry	x	y	z	q	α ($Å^3$)[a]
R	16(c)	D_{3d}	0	0	0	3	α_R
Ti	16(d)	D_{3d}	1/2	1/2	1/2	4	0.22
O_1	8(a)	T_d	1/8	1/8	1/8	-2	1.349
O_2	48(f)	C_{2v}	x	1/8	1/8	-2	1.349
X	8(b)	T_d	3/8	3/8	3/8	--	--

[a]Reference 5.

29.2 X-Ray Data on $R_2Ti_2O_7$ (reference 4) and Polarizabilities, α_R, of Rare Earth Ions, R^{3+} ($4f^N$) (reference 3)

N	R	a (Å)	x	α_R ($Å^3$)
5	Sm	10.2303	0.4230	1.11
6	Eu	10.1988	--	1.06
7	Gd	10.1857	0.4263	1.01
8	Tb	10.1560	--	0.97
9	Dy	10.1245	--	0.94
10	Ho	10.0979	--	0.90
11	Er	10.0759	0.4194	0.86
12	Tm	10.0533	--	0.83
13	Yb	10.0309	0.4201	0.80
14	Lu	10.0258	--	0.77

29.3 Crystal-Field Components, A_{nm}

Crystal-field components were obtained for R = Sm, Gd, Er, and Yb. A least-squares polynomial fit was used to obtain the components for the entire range of R. In 29.3.1 to 29.3.12, the crystal is rotated so that the z-axis is parallel to the (111) crystallographic axis.

29.3.1 A_{20} ($cm^{-1}/Å^2$) for R site 16c (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	8047.5	-1157.9	396.60	8759.2
Eu	8118.3	-1168.8	392.06	6298.6
Gd	8180.3	-1175.9	387.70	4446.7
Tb	8233.2	-1179.3	383.53	3203.4
Dy	8277.3	-1178.8	379.54	2568.9
Ho	8312.5	-1174.6	375.73	2543.1
Er	8338.7	-1166.6	372.10	3125.9
Tm	8356.0	-1154.8	368.66	4317.5
Yb	8364.4	-1139.2	365.41	6117.8
Lu	8363.8	-1119.8	362.33	8526.7

29.3.2 A_{40} ($cm^{-1}/Å^4$) for R site 16c (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	8,295.2	-2797.7	22.651	8132.0
Eu	9,564.4	-2854.0	27.268	8213.1
Gd	10,594	-2913.0	34.538	8296.4
Tb	11,384	-2974.6	44.460	8382.0
Dy	11,934	-3038.7	57.034	8469.8
Ho	12,245	-3105.5	72.261	8559.8
Er	12,316	-3174.9	90.141	8652.1
Tm	12,148	-3246.8	110.67	8746.6
Yb	11,740	-3321.4	133.86	8843.4
Lu	11,092	-3398.6	159.09	8942.3

29.3.3 A_{43} ($cm^{-1}/Å^4$) for R site 16c (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	2378.8	-569.66	-1038.3	770.73
Eu	2405.2	-580.49	-1055.5	769.11
Gd	2454.3	-596.22	-1087.6	770.41
Tb	2526.1	-616.84	-1134.6	774.63
Dy	2620.5	-642.35	-1196.4	781.76
Ho	2737.6	-672.75	-1273.1	791.80
Er	2877.4	-708.05	-1364.6	804.76
Tm	3039.9	-748.24	-1471.0	820.64
Yb	3225.0	-793.33	-1592.2	839.44
Lu	3432.8	-843.31	-1728.3	861.15

29.3.4 A_{60} ($cm^{-1}/Å^6$) for R site 16c (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	1750.0	-840.62	-56.417	852.93
Eu	1781.8	-862.76	-59.013	860.01
Gd	1815.3	-885.71	-63.115	866.49
Tb	1850.6	-909.45	-68.724	872.38
Dy	1887.5	-934.00	-75.838	877.66
Ho	1926.2	-959.36	-84.457	882.35
Er	1966.6	-985.51	-94.583	886.45
Tm	2008.7	-1012.5	-106.21	889.94
Yb	2052.5	-1040.2	-119.35	892.84
Lu	2098.0	-1068.8	-134.00	895.14

29.3.5 A_{63} ($cm^{-1}/Å^6$) for R site 16c (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	-698.03	198.07	182.45	-317.52
Eu	-709.98	203.77	186.39	-319.83
Gd	-726.15	211.36	193.04	-321.76
Tb	-746.55	220.85	202.40	-323.31
Dy	-771.17	232.23	214.47	-324.48
Ho	-800.02	245.51	229.25	-325.28
Er	-833.10	260.69	246.73	-325.70
Tm	-870.40	277.76	266.93	-325.74
Yb	-911.93	296.73	289.83	-325.40
Lu	-957.69	317.59	315.44	-324.69

29.3.6 A_{66} ($cm^{-1}/Å^6$) for R site 16c (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	1014.0	-306.71	-147.86	477.36
Eu	1031.3	-314.60	-150.90	641.04
Gd	1052.3	-324.46	-155.96	735.96
Tb	1076.8	-336.29	-163.05	762.13
Dy	1105.0	-350.09	-172.16	719.55
Ho	1136.8	-365.87	-183.31	608.21
Er	1172.3	-383.62	-196.48	428.11
Tm	1211.3	-403.35	-211.68	179.25
Yb	1254.0	-425.05	-228.91	-138.35
Lu	1300.3	-448.72	-248.16	-524.72

29.3.7 A_{20} ($cm^{-1}/Å^2$) for Ti site 16d (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	-13,382	1444.3	12,981	1043.4
Eu	-13,282	1441.8	13,035	1195.7
Gd	-13,476	1461.6	13,172	1158.1
Tb	-13,965	1503.7	13,391	930.45
Dy	-14,748	1568.2	13,692	512.83
Ho	-15,826	1655.0	14,076	-94.792
Er	-17,199	1764.2	14,542	-892.41
Tm	-18,866	1895.7	15,090	-1880.0
Yb	-20,828	2049.5	15,720	-3057.6
Lu	-23,084	2225.7	16,432	-4425.2

29.3.8 A_{40} ($cm^{-1}/Å^4$) for Ti site 16d (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	-15,449	5539.2	-4263.2	-14,173
Eu	-15,682	5671.4	-4302.6	-14,313
Gd	-15,823	5761.3	-4388.2	-14,450
Tb	-15,872	5809.0	-4520.0	-14,584
Dy	-15,830	5814.5	-4698.0	-14,714
Ho	-15,696	5777.7	-4922.3	-14,841
Er	-15,471	5698.6	-5192.8	-14,965
Tm	-15,153	5577.4	-5509.5	-15,086
Yb	-14,744	5413.8	-5872.4	-15,203
Lu	-14,244	5208.1	-6281.5	-15,317

29.3.9 A_{43} ($cm^{-1}/Å^4$) for Ti site 16d (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	21,584	-8272.2	2158.6	15,464
Eu	21,851	-8445.4	2185.6	15,596
Gd	22,079	-8593.4	2245.2	15,743
Tb	22,268	-8716.2	2337.2	15,906
Dy	22,417	-8814.0	2461.7	16,084
Ho	22,527	-8886.5	2618.7	16,279
Er	22,597	-8933.9	2808.2	16,489
Tm	22,628	-8956.1	3030.2	16,715
Yb	22,619	-8953.1	3284.7	16,956
Lu	22,571	-8925.0	3571.7	17,213

$R_2Ti_2O_7$

29.3.10 A_{60} ($cm^{-1}/Å^6$) for Ti site 16d (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	3912.5	-2792.4	29.807	1149.9
Eu	3968.2	-2853.9	32.760	1147.0
Gd	4026.5	-2914.2	47.133	1159.4
Tb	4087.6	-2973.5	72.926	1187.0
Dy	4151.3	-3031.6	110.14	1229.8
Ho	4217.7	-3088.5	158.77	1287.9
Er	4286.8	-3144.3	218.82	1361.2
Tm	4358.6	-3199.0	290.30	1449.8
Yb	4433.0	-3252.5	373.19	1553.6
Lu	4510.2	-3304.9	467.50	1672.6

29.3.11 A_{63} ($cm^{-1}/Å^6$) for Ti site 16d (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	-150.68	-9.2581	1199.2	1039.2
Eu	-132.98	-26.031	1213.1	1054.1
Gd	-143.99	-20.254	1231.8	1067.6
Tb	-183.69	8.0703	1255.3	1079.7
Dy	-252.09	58.943	1283.6	1090.4
Ho	-349.20	132.36	1316.7	1099.9
Er	-475.00	228.33	1354.6	1107.9
Tm	-629.51	346.85	1397.3	1114.6
Yb	-812.72	487.92	1444.8	1120.0
Lu	-1024.6	651.53	1497.1	1124.0

29.3.12 A_{66} ($cm^{-1}/Å^6$) for Ti site 16d (D_{3d})

R	Monopole	Self-induced	Dipole	Total
Sm	2346.3	-1665.6	-70.846	609.77
Eu	2384.7	-1706.3	-70.685	607.71
Gd	2425.9	-1747.3	-69.591	609.02
Tb	2469.9	-1788.6	-67.564	613.71
Dy	2516.7	-1830.2	-64.606	621.78
Ho	2566.2	-1874.2	-60.714	633.22
Er	2618.5	-1914.6	-55.890	648.03
Tm	2673.6	-1957.2	-50.134	666.22
Yb	2731.5	-2000.2	-43.445	687.79
Lu	2792.2	-2043.5	-35.824	712.73

29.3.13 A_{32} ($cm^{-1}/Å^3$) for vacancy site, X, 8b (T_d)

R	Monopole	Self-induced	Dipole	Total
Sm	-36,871	-538.71	606.15	-36,804
Eu	-37,235	-549.82	612.32	-37,174
Gd	-37,617	-560.68	625.71	-37,553
Tb	-38,017	-571.30	646.31	-37,944
Dy	-38,435	-581.67	674.14	-38,344
Ho	-38,871	-591.80	709.18	-38,756
Er	-39,325	-601.69	751.44	-39,177
Tm	-39,798	-611.33	800.91	-39,610
Yb	-40,288	-620.73	857.61	-40,053
Lu	-40,796	-629.89	921.52	-40,506

29.3.14 A_{40} ($cm^{-1}/Å^4$) for vacancy site, X, 8b (T_d)

R	Monopole	Self-induced	Dipole	Total
Sm	34,671	-6813.8	4,549.7	33,401
Eu	35,195	-7002.9	3,407.7	33,797
Gd	35,598	-7125.0	2,704.2	34,162
Tb	35,877	-7180.0	2,439.2	34,496
Dy	36,035	-7168.0	26,12.6	34,798
Ho	36,071	-7089.0	3,224.5	35,069
Er	35,984	-6943.0	4,274.9	35,308
Tm	35,775	-6729.9	5,763.8	35,517
Yb	35,444	-6449.9	7,691.1	35,694
Lu	34,991	-6102.8	10,057	35,839

29.3.15 A_{44} ($cm^{-1}/Å^4$) for vacancy site, X, 8b (T_d)

R	Monopole	Self-induced	Dipole	Total
Sm	20,719	-4071.9	3313.3	19,961
Eu	21,033	-4185.0	3349.0	20,198
Gd	21,274	-4257.9	3399.0	20,415
Tb	21,441	-4290.8	3463.5	20,614
Dy	21,536	-4283.7	3542.4	20,795
Ho	21,557	-4236.4	3635.6	20,957
Er	21,505	-4149.2	3743.2	21,100
Tm	21,380	-4021.9	3865.2	21,224.0
Yb	21,181	-3854.5	4001.6	21,330
Lu	20,910	-3647.0	4152.4	21,418

29.3.16 A_{60} ($cm^{-1}/Å^6$) for vacancy site, X, 8b (T_d)

R	Monopole	Self-induced	Dipole	Total
Sm	-494.90	-807.28	405.60	896.57
Eu	-496.57	-834.96	412.24	-919.25
Gd	-508.14	-853.75	419.91	-941.93
Tb	-529.63	-863.66	428.60	-964.63
Dy	-561.02	-864.68	438.31	-987.33
Ho	-602.32	-856.83	499.05	-1010.0
Er	-653.53	-840.09	460.81	-1032.8
Tm	-714.64	-814.48	473.59	-1055.5
Yb	-785.67	-779.98	487.39	-1078.2
Lu	-866.60	-736.60	502.22	-1101.0

29.3.17 A_{64} ($cm^{-1}/Å^6$) for vacancy site, X, 8b (T_d)

R	Monopole	Self-induced	Dipole	Total
Sm	925.92	1510.2	-758.83	1677.3
Eu	929.02	1562.0	-771.26	1719.7
Gd	950.66	1597.2	-785.60	1762.2
Tb	990.84	1615.8	-801.86	1804.7
Dy	1049.6	1617.7	-820.03	1847.2
Ho	1126.8	1603.0	-840.12	1889.6
Er	1222.6	1571.7	-862.11	1932.1
Tm	1336.9	1523.7	-886.03	1974.6
Yb	1469.8	1459.1	-911.85	2017.1
Lu	1621.2	1377.9	-939.56	2059.6

29.3.18 A_{72} ($cm^{-1}/Å^7$) for vacancy site, X, 8b (T_d)

R	Monopole	Self-induced	Dipole	Total
Sm	1034.2	57.289	-0.264	1091.2
Eu	1055.0	58.860	-0.263	1113.6
Gd	1076.4	60.479	-0.258	1136.5
Tb	1098.2	62.148	-0.249	1160.0
Dy	1120.5	63.867	-0.237	1184.0
Ho	1143.2	65.635	-0.220	1208.6
Er	1166.5	67.452	-0.199	1233.7
Tm	1190.3	69.319	-0.174	1259.4
Yb	1214.6	71.236	-0.145	1285.6
Lu	1239.3	73.201	-0.112	1312.4

29.3.19 A_{76} ($cm^{-1}/Å^7$) for vacancy site, X, 8b (T_d)

R	Monopole	Self-induced	Dipole	Total
Sm	951.31	52.697	-0.243	1003.8
Eu	970.47	54.142	-0.242	1024.4
Gd	990.07	55.632	-0.238	1045.5
Tb	1010.1	57.167	-0.230	1067.1
Dy	1030.6	58.748	-0.218	1089.2
Ho	1051.6	60.374	-0.202	1111.8
Er	1073.0	62.046	-0.183	1134.9
Tm	1094.9	63.763	-0.160	1158.5
Yb	1117.2	65.526	-0.133	1182.6
Lu	1139.9	67.334	-0.102	1207.2

29.4 Experimental Parameters (cm^{-1}) (reference 1)

nd^N	Ion	$F^{(2)}$	$F^{(4)}$	B_{40}^a
$3d^2$	V^{3+}	63,903	41,378	-24,500
$3d^3$	Cr^{3+}	65,450	42,840	-26,222
$3d^3$	Mn^{4+}	--	--	-31,920
$3d^4$	Mn^{3+}	--	--	-28,406
$3d^6$	Co^{3+}	58,100	34,902	-24,360
$3d^7$	Co^{2+}	66,220	43,344	-8,442
$3d^7$	Ni^{3+}	--	--	--
$3d^8$	Ni^{2+}	84,420	61,110	-12,278

$^aB_{43} = \sqrt{10/7}\,|B_{40}|$

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30. $Y_2Ti_2O_7$

30.1 Crystallographic Data on $Y_2Ti_2O_7$ for Two Choices of Ion Sites

30.1.1 Cubic O_h^7 (Fd3m), 227 (second setting), Z = 8 (see reference 4)

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)[b]
Y	16(c)	D_{3d}	0	0	0	3	0.870
Ti	16(d)	D_{3d}	1/2	1/2	1/2	4	0.22[c]
O_1	8(a)	T_d	1/8	1/8	1/8	-2	1.349
O_2	48(f)	C_{2v}	0.4201	1/8	1/8	-2	1.349
X	8(b)	T_d	3/8	3/8	3/8	0	0

[a]X-ray data: a = 10.095 Å (reference 4).
[b]Reference 6.
[c]Reference 3.

30.1.2 Cubic O_h^7 (Fd3m), 227 (second setting), Z = 8 (see reference 2)

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)[b]
Y	16(d)	D_{3d}	1/2	1/2	1/2	3	0.870
Ti	16(c)	D_{3d}	0	0	0	4	0.22[c]
O_1	8(b)	T_d	3/8	3/8	3/8	-2	1.349
O_2	48(f)	C_{2v}	-0.0788	1/8	1/8	-2	1.349
X	8(a)	T_d	1/8	1/8	1/8	0	0

[a]X-ray data: a = 10.0896 Å (reference 2).
[b]Reference 6.
[c]Reference 3.

30.2 Crystal-Field Components, A_{nm}

The crystal-field components, A_{nm} ($cm^{-1}/Å^n$), are calculated through n = 6 because of the possibility of rare-earth ions occupying these sites.

30.2.1 For Y ion in 16c (D_{3d}) site of reference 4 (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	8,240.0	-1128.5	364.00	7475.8
A_{40}	11,645	-3144.5	109.33	8610.3
A_{43}	3,006.4	-730.62	-1446.6	829.14
A_{60}	1,953.6	-972.14	-103.67	877.82
A_{63}	-850.91	268.34	260.36	-322.20
A_{66}	1,181.5	-389.33	-206.36	585.85

30.2.2 For Ti ion in 16d (D_{3d}) site of reference 4 (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	-19,051	1887.4	14,909	-2,255.2
A_{40}	-14,726	5340.5	-5,416.7	-1,4802
A_{43}	22,131	-8635.8	2,984.9	16,480
A_{60}	4,242.0	-3071.0	292.87	1,463.5
A_{63}	-651.50	363.80	1,355.4	1,067.7
A_{66}	2,602.1	-1878.9	-47.720	675.50

30.2.3 For vacancy site, X, 8b (T_d) of reference 4

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{32}	-39,176	592.38	-790.43	38,978
A_{40}	34,880	-6419.5	6321.3	34,782
A_{44}	-20,845	3836.4	-3777.7	-20,786
A_{60}	-708.11	-769.29	458.09	-10,19.3
A_{64}	1,324.7	1439.2	-857.02	1,906.9
A_{72}	-1,152.4	-66.33	0.164	-1,218.6
A_{76}	1,060.1	61.01	-0.151	1,127.0

30.2.4 For Y ion in 16d (D_{3d}) site of reference 2 (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	8,287.8	-1156.5	387.95	7519.2
A_{40}	11,686	-3152.3	83.620	8616.9
A_{43}	2,885.0	-704.81	-1367.9	812.26
A_{60}	1,951.9	-974.79	-92.36	884.77
A_{63}	-830.75	258.58	246.83	-325.34
A_{63}	1,167.4	-380.73	-196.75	589.93

30.2.5 For Ti ion 16c (D_{3d}) site of reference 2 (rotated so that z-axis is parallel to (111) crystallographic axis)

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	-17,718	1800.6	14,730	-1,187.9
A_{40}	-15,256	5588.2	-5,256.1	-14,924.11
A_{43}	22,458	-8832.3	2,832.7	16,458
A_{60}	4,281.6	-3127.7	221.09	1,374.9
A_{63}	-528.42	271.33	1,370.2	1,113.2
A_{66}	26,070	-1898.32	-57.96	650.70

30.2.6 For vacancy site, X'', 8a (T_d) of reference 2

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{32}	39,189	596.74	-757.44	39,028
A_{40}	35,555	-6746.5	6306.3	35,114.626
A_{44}	-21,248	4031.8	-3768.8	-20,985
A_{60}	-668.40	-812.34	462.050	-1,018.7
A_{64}	1,250.5	1519.7	-864.417	1,905.8
A_{72}	-1,157.4	-66.723	0.208	-1,223.9
A_{76}	1,064.6	61.376	-0.191	1,125.8

30.3 Experimental Parameters (cm^{-1}) (reference 1)

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	B_{40}
V^{3+}	$3d^2$	63,217	41,378	-23,590
Cr^{3+}	$3d^3$	59,444	38,909	-25,970
Mn^{3+}	$3d^4$	--	--	-28,168
Co^{3+}	$3d^6$	56,630	34,020	-23,730
Mn^{4+}	$3d^3$	--	--	-31,822
Co^{2+}	$3d^7$	65,835	43,092	-8,330
Ni^{2+}	$3d^8$	84,420	61,110	-12,180

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K_2ReCl_6

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31. K_2ReCl_6

31.1 Crystallographic Data on K_2ReCl_6

Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x^a	y	z	q	α (A^3)
Re	4a	O_h	0	0	0	4	0.70^b
K	8c	T_d	1/4	1/4	1/4	1	0.827^c
Cl	24e	C_{4v}	x	0	0	-1	2.694^c

[a]X-ray data: a = 9.861 A, x = 0.240 (reference 5).
[b]Reference 3.
[c]Reference 4.

31.2 Crystal-field Components, A_{nm} (cm^{-1}/A^n), for Re (O_h) Site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{40}	5793.3	-4601.3	9735.1	10,927
A_{44}	3462.2	-2749.8	5817.9	6,530.2

31.3 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}	Ref
Re^{4+}	$5d^3$	31,891	20,928	2328	90,564	2

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32. A_2BF_6 (A = K, Rb, Cs; B = Ge, Zr)

32.1 Crystallographic Data on A_2BF_6

Hexagonal D_{3d}^3 ($P\bar{3}m1$), 164, Z = 1

Ion	Site	Symmetry	x	y	z	q	α ($Å^3$)
B	1(a)	D_{3d}	0	0	0	4	α_B
A	2(d)	C_{3v}	1/3	2/3	z	1	α_A
F	6(i)	C_s	x	-x	z	-1	0.731

32.2 X-Ray Data

A	B	a (Å)[a]	c (Å)	z_A	x_F	z_F	α_A ($Å^3$)[b]	α_B ($Å^3$)[c]
K	Ge	5.62	4.65	0.70	0.148	0.220	0.827	0.12
Rb	Ge	5.82	4.79	0.695	0.144	0.213	1.383	0.12
Cs	Zr	6.41	5.01	0.692	0.16	0.198	2.492	0.48
Rb	Zr	6.16	4.82	0.691	0.167	0.206	1.383	0.48

[a]Reference 7.
[b]Reference 6.
[c]Reference 4.

32.3 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$)

32.3.1 For Ge (D_{3d}) site of K_2GeF_6

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	3,371.0	-52.7	-2,040.3	1,277.9
A_{40}	-15,618	8,667.1	-18,481	-25,432
A_{43}	19,236	-10,270	23,136	32,103

32.3.2 For Ge site (D_{3d}) site of Rb_2GeF_6

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	2,187.4	89.8	-2,279.8	-2.610
A_{40}	-15,138	8310.5	-17,768	-24,595
A_{43}	18,831	-9956.6	22,422	31,296

32.3.3 For Zr (D_{3d}) site of Cs_2ZrF_6

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	-10,846	1089.7	-4014.2	-13,771
A_{40}	-5,354.3	1942.2	-4819.3	-8,231.4
A_{43}	9,810	-3407.0	8328.6	14,732

32.3.4 For Zr (D_{3d}) site of Rb_2ZrF_6

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	-11,003	1047.3	-3653.0	-13,608
A_{40}	-5,288.4	1888.9	-4747.9	-8,147.4
A_{43}	9,737.6	-3347.2	8207.6	14,598

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33. Rb_2SnCl_6

33.1 Crystallographic Data on Rb_2SnCl_6

Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x^a	y	z	q	α ($Å^3$)
Sn	4(a)	O_h	0	0	0	4	0.37^b
Rb	8(c)	T_d	1/4	1/4	1/4	1	1.383^c
Cl	24(e)	C_{4v}	x	0	0	-1	2.694^c

[a]X-ray data: a = 10.118 Å, x = 0.240 (reference 12).
[b]Reference 7.
[c]Reference 8.

33.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$), for Sn (O_h) Site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{40}	5094.0	-3739.2	8166.3	9521.1
A_{44}	3044.3	-2234.6	4880.3	5689.9

33.3 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}	Ref
Os^{4+}	d^4	28,549	17,365	2606	40,198	9

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34. Cs_2TeCl_6

34.1 Crystallographic Data on Cs_2TeCl_6

Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x[a]	y	z	q	α [Å^3)
Te	4(a)	O_h	0	0	0	4	1.21[b]
Cs	8(c)	T_d	1/4	1/4	1/4	1	2.492[c]
Cl	24(e)	C_{4v}	x	0	0	-1	2.694[c]

[a]X-ray data: a = 10.447 Å, x = 0.240.
[b]Reference 5.
[c]Reference 6, reference 8.

34.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$) for Te (O_h) Site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{40}	4340.9	-2885.2	6549.2	8004.9
A_{44}	2594.2	-1724.2	3913.9	4783.9

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35. K_2ReF_6

35.1 Crystallographic Data on K_2ReF_6

Hexagonal D_{3d}^3 ($P\bar{3}m1$), 164, Z = 1

Ion	Site	Symmetry	x^a	y	z	q	α (Å^3)
Re	1(a)	D_{3d}	0	0	0	4	0.70[b]
K	2(d)	C_{3v}	1/3	2/3	0.3007	1	0.827[c]
F	6(i)	Cs	0.1617	-0.167	0.2276	-1	0.731[c]

[a]X-ray data: a = 5.879 Å, c = 4.611 Å (reference 2).
[b]Reference 3.
[c]Reference 4.

35.2 Crystal-Field Components, A_{nm} (cm^{-1}/Å^n), for Re (D_{3d}) Site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{20}	-4,231	592.3	-2741	-6380
A_{40}	-8,445	3421	-7791	-12815
A_{43}	-12,038	4732	-11291	-18597

35.3 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	ζ	B_{20}	B_{40}	B_{43}	Ref
Re^{4+}	$5d^3$	41,076	25,409	2612	-7136	-33,993	44,925	1

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36. Cs_2ZrCl_6

36.1 Crystallographic Data on Cs_2ZrCl_6

Cubic O_h^5 (Fm3m), 225, Z = 4

Ion	Site	Symmetry	x[a]	y	z	q	α (Å³)
Zr	4(a)	O_h	0	0	0	4	0.48[b]
Cs	8(c)	T_d	1/4	1/4	1/4	1	2.492[c]
Cl	24(e)	C_{4v}	x	0	0	-1	2.694[c]

[a]X-ray data: a = 10.407 Å, x = 0.235 (reference 13).
[b]Reference 6.
[c]Reference 11.

36.2 Crystal-Field Components, A_{nm} ($cm^{-1}/Å^n$), for Zr (O_h) Site

A_{nm}	Monopole	Self-induced	Dipole	Total
A_{40}	4883.9	-3524.3	7742.1	9101.6
A_{44}	2918.7	-2106.2	4626.8	5439.3

36.3 Experimental Parameters (cm^{-1})

Ion	nd^N	$F^{(2)}$	$F^{(4)}$	ζ	B_{40}	Ref.
Ru^{4+}	$4d^4$	48,888	17,173	1044	39,732	9
Re^{4+}	$5d^3$	28,749	22,906	2392	63,729	5
Os^{4+}	$5d^4$	45,381	16,329	2416	47,229	4

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